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Ultra-Cold Atoms, Ions, Molecules and Quantum Technologies

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Preamble

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Forty years ago, twenty years after the discovery of the laser, physicists were developing laser cooling methods for ions trapped in electromagnetic fields. From the 1980s onwards, these techniques were refined and extended to atoms, thanks to the audacity and inventiveness of a generation of pioneering researchers. Actually, it was necessary to succeed simultaneously in trapping and cooling samples of atomic gases in a vacuum at a distance from any wall. Spectacular results followed and extraordinarily low temperatures were quickly reached, very close to absolute zero. The field of “cold atoms” was born, rewarded by successive Nobel prizes, first of which was awarded in 1997 to William D. Phillips, Steven Chu and Claude Cohen–Tannoudji, last in 2022 to Alain Aspect. Gaseous samples of a few thousand to a few billion atoms can be prepared at a few millionths of a degree above absolute zero, which means that the particles move at extremely low speed, of the order of centimetres per second. At these extreme temperatures, the behaviour of matter changes and its properties can only be described using quantum mechanics and the wave properties of particles. New physical phenomena have been discovered and innovations have followed the theoretical and experimental progress of the research. Initially imagined as a wonderful method for perfecting atomic physics, cold atoms have gradually proved to be powerful tools for research in cross-cutting fields of physics, such as condensed matter and even high-energy physics. These atoms are now referred to as ‘quantum gases’ at such low temperatures that their collective behaviour is modified by the laws of quantum mechanics.

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The field of quantum gases began in the United States and Europe and has since grown dramatically around the world. Today, it continues to attract successive generations of the brightest students from all countries. This continuing success is partly due to the flexibility of the studies that each experiment allows: the density of the gas, its temperature, the geometry of the samples, the strength of the interactions between the particles, etc. can be varied. The set-ups are certainly quite complex, but remain on a human scale, allowing everyone to learn mastering many techniques. In addition, the field of quantum gases generally combines theory and experiment, which is an additional attraction for the researcher who likes to understand the whole subject. Nowadays, cold atoms are like lasers. On the one hand, they are still objects of study that research is trying to perfect: the limit of extreme temperatures is being pushed back further and further to the vicinity of absolute zero, densities are being varied from a few billion atoms per cm^3 to a few isolated atoms, the range of cooled particles (atoms, ions, molecules, clusters, etc.) is being extended, and devices are being miniaturized and simplified. On the other hand, quantum gases provide usable tools to try to understand more and more complex phenomena such as N-body physics or quantum transport, as well as to explore the conceptual foundations of quantum mechanics. They are part of what is known as the second quantum revolution, which results from the possibility of isolating and visualizing single particles (atoms, ions, photons, etc.), and also of implementing the phenomena of quantum entanglement, the basic concept of quantum mechanics. Quantum gases are thus well positioned in the emerging field of quantum technologies, which is currently the subject of a spectacular global effort, particularly in Europe where the European Union has been deploying a flagship programme with significant resources since 2017.

The book presents the most recent developments in quantum gas physics. As a follow-up to Erwan Jahier's "Cold atoms" published in 2010 in the same collection, it traces the exceptional growth of the field over the last ten years. The book explores the multiple axes along which this field of research unfolds, without aiming at an impossible exhaustiveness. Each chapter is written by one or more authors, all of whom are active researchers. They describe in pedagogical but precise terms the state of progress of research in their field. The whole book is coordinated by three researchers who ensure its coherence.

After a brief review of the physics of the interaction of atoms with light, the first chapter describes the succession of methods that made it possible to produce and understand the cooling of dilute gases to extremely low temperatures and to trap these gaseous samples levitating in vacuum. This chapter also reminds the first major breakthrough, the experimental demonstration of Bose–Einstein condensation. Chapter 2 is devoted to the very significant advances in physics metrology that cooled quantum systems have enabled. There has been steady progress in the accuracy of atomic clocks in the microwave and then optical range, which is of particular importance for the future definition of the second. Other types of cold atom instruments such as interferometers are also maturing. This opens up new possibilities to probe the fundamental laws of physics. Chapter 3 shows how the increasing control of atomic cooling, quantum states of light and the interaction between light and matter have found a new field of application in recent years with quantum information networks. The linear and non-linear operations required for the storage and processing of quantum information are described in this chapter and how cold atoms have made it possible to develop various efficient devices. Chapter 4 details the possibilities opened up by quantum gases in the field of quantum simulation. The aim is to answer questions raised by the physics of systems consisting of many interacting quantum objects with the help of another, more easily manipulated quantum system, such as cold atoms assembled in optical lattices, or trapped one by one by optical tweezers and arranged to form artificial crystals. Applications include quantum magnetism and superconductivity. Chapter 5 deals with wave scattering and disorder from a theoretical point of view. Cold atoms can play the role of these scattered waves when immersed in a disordered optical medium. In the field of transport, the effect of disorder is specifically taken into account even in the presence of interactions between particles. Situations where disorder makes it impossible to return to equilibrium are also described.

Chapter 6 extends the physics of cooled quantum gases to ions. The trapping methods are different from those for cold atoms, but many applications are common: precision measurements, spectroscopy, collision studies, quantum simulation and information. Cooled ions are also the tools of choice for fundamental experiments such as antimatter research. Finally, chapter 7 extends cooling methods to molecules. Cold molecules can be obtained by combining cold atoms by various optical or magnetic methods. Recently, alternative methods for direct cooling of molecules to temperatures as low as those achievable with atoms have also been developed. The applications are diverse, ranging from quantum simulation and information to the control of chemical reactions. Cold molecules also open the way to new tests of fundamental physics. This book as a whole is designed for anyone interested in science and technology. It is aimed in particular at students in preparatory classes and at undergraduate and graduate students. It may also be useful to young – and not so young – researchers who are approaching the field of quantum physics, and to all those who are interested in quantum technologies, a subject that is in full development. The book contains very few equations, but many figures, sketches and colour illustrations that make it attractive and relatively easy to read. It aims to share with a wide audience the passion that drives all the authors, all of whom actively engaged in their research.

Coordinators, Contributors, Sponsors and Acknowledgments

The Coordinators

The present book is collectively written by nineteen researchers whose names are recorded at the head of each chapter and given below. Coordination of this book has been done by Robin Kaiser, Michèle Leduc, and Hélène Perrin.

Robin Kaiser

Robin Kaiser is a research director at CNRS. He started his career in atomic physics at École normale supérieure with a PhD thesis under the supervision of Alain Aspect, in the group led by Claude Cohen–Tannoudji. He then did a postdoctoral stay at Harvard University in Gerald Gabrielse's group, before joining Alain Aspect as a research fellow at CNRS to start a new activity in cold atoms at the Institut d'Optique. Since 1996, Robin Kaiser is heading the cold atoms team at the Institut de Physique de Nice. His research work focuses on light scattering by cold atoms, combining cold atom physics with mesoscopic physics, and localization of light and quantum optics. He has initiated studies of intensity correlations in astrophysics, taking up the historical studies of Hanbury–Brown and Twiss with the modern tools of quantum optics. He is also the director of the "Cold atoms" GDR (French research network) since its creation.

Michèle Leduc

Michèle Leduc is a research director emeritus at CNRS. Her career in atomic physics was mainly spent at the École normale supérieure in Paris, in the Laboratoire Kastler Brossel named after its founders Alfred Kastler (Nobel laureate in 1966) and Jean Brossel. In 1993 she joined the laser cooling team led by Claude Cohen Tannoudji, Nobel laureate in 1997. Her most recent research work focuses on Bose–Einstein condensates of metastable helium. She coordinated the outreach activities of SIRTEQ, the research network on quantum technologies in the Ile-de-France region up to late 2021. She is editor of science books for the CNRS and for EDP-Sciences. She was a member of the CNRS Ethics Committee (COMETS) from 2012 to 2021.

Hélène Perrin

Hélène Perrin is a research director at CNRS. She prepared a PhD thesis at the Laboratoire Kastler Brossel under the supervision of Christophe Salomon on laser cooling of atoms in an optical trap. She did a postdoctoral stay at the CEA on two-dimensional electron gases with Christian Glattli. She then was recruited as a research fellow by CNRS at the Laboratoire de physique des lasers at Paris Nord University, where she currently leads the BEC team. Her research focuses on Bose–Einstein condensates confined in radio frequency traps and more specifically on their superfluid properties. She teaches at the École normale supérieure and at the University of Paris. She is regularly invited to give lectures in international summer schools such as the Physics School at Les Houches. She coordinated the Quantum Simulation axis of the SIRTEQ network together with Pascal Simon and is a board member of the "Cold atoms" French research network. She is now head of QuanTip, the new research network on quantum technologies in Ile-de-France.

The contributors

The researchers who wrote the different chapters of this book are: Baptiste Allard, Juliette Billy, Nadia Bouloufa-Maafa, Nicolas Cherroret, Daniel Comparat, Olivier Dulieu, Laurent Hilico, Vincent Josse, Robin Kaiser, Martina Knoop, Bruno Laburthe, Thierry Lahaye, Michèle Leduc, Hans Lignier, Jérôme Lodewyck, Franck Pereira dos Santos, Hélène Perrin, Goulven Quemener, Jakob Reichel. These researchers work in CNRS laboratories most of them associated to various universities. The coordinators thank all the authors for their kind cooperation to the present collective enterprise.

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Cold Atom GDR

The "Cold atoms" GDR network was created in 2012. This network of more than 20 laboratories across France coordinates activities in the field of cold atoms in France, structures the training of young PhD students, organizes meetings and conferences, distributes resources and contributes to the influence of the field.

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Preface

Fifteen miraculous years: bypassing impossibility theorems

Alain Aspect

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When Michèle, Hélène and Robin asked me to write a preface for this book, it was impossible for me to refuse, but I found it difficult to embark on the somewhat conventional exercise of saying something positive about each chapter, even though reading them convinced me of their exceptional quality. In fact, this reading made me realize that cold atoms, once an object of advanced research, have become today a tool for multiple applications in the field of fundamental research and quantum technologies, of which this book gives a good sample. Thinking of the potential readers — the general public curious about the current developments of science, but also students engaged in a master or even a thesis using cold atoms — I thought it would be a pity if they were totally unaware of the exciting adventure we all experienced in developing this tool. I therefore decided to share with them some memories of the emergence of this field as it matured. I had the privilege of participating at the Cold Atoms group of Collège de France and Laboratoire Kastler Brossel (LKB) of the École normale supérieure in paris, and then at the Laboratoire Charles Fabry de l'Institut d'Optique in Orsay and Palaiseau.

So here are some personal memories of the early years of laser cooling of atoms leading to the gaseous Bose–Einstein condensates, the basic tools for the wonderful applications described in this book. This is not a tutorial of science history, but it recalls how I experienced this history, or more exactly what I remember. It is biased by the places from which I observed it, and above all by my own obsessions: forgetting nothing of the mistakes and disappointments, the good ideas and the lucky

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breaks, by putting them in the context of the evolution of the great concepts of physics. I hope that it may be a useful lesson for young physicists who are starting out in the field, and that it can interest the "curious amateurs" who should not believe that scientific discovery is a long quiet river. During these fifteen years, from 1985 to 2000, several barriers considered as ultimate limits were overcome, or rather bypassed. The lesson is obvious: one should not be stopped by impossibility theorems without double thinking about them. There might exist situations where these no-go theorems do not apply, that can be discovered by theoretical reflection or, more often, by doing experiments, letting Nature show the way to those who can see it. One should not underestimate the role of luck, the so-called "serendipity", from which we happen to find better than what we looked for.

The years 1985–1988 were extraordinary.[1] In the autumn of 1985, the "cold atoms" team of the Kastler Brossel Laboratory and Collège de France around Claude Cohen–Tannoudji — the three 'musketeers' Jean Dalibard, Christophe Salomon and myself—was hard at work. Our first apparatus was quite modest compared to the sophisticated set-ups of today: an atomic beam of cesium, a laser diode to act on the transverse distribution of the atomic velocities, and a hot wire detector to analyze the profile of the beam after two meters of propagation. We were plotting the results point by point, by hand, on graph paper; Claude was in charge of such plots when he spent time with us in the laboratory. We were trying to demonstrate "blue molasses cooling", a new mechanism for cooling atoms with lasers detuned from the atomic resonance to the short wavelength side.[2] The idea came from the dressed atom model used by Jean and Claude to give a simple image of the dipole force, one of the two radiative forces. It was the first occurrence of what we would call later the "Sisyphus effect". Then we received the tremendous news that the Bell Labs team—Steven Chu, Arthur Ashkin and their colleagues—had succeeded at keeping atoms "stuck" for a fraction of a second in an optical molasses, at the intersection of three pairs of lasers "red" detuned below the atomic resonance frequency.

The idea had been proposed ten years earlier by Theodor Hänsch and Arthur Schawlow, considering that the resonant pressure force, the other radiative force,[3] varied with the atom velocity: this was therefore called "Doppler cooling". With six waves detuned below the atomic resonance frequency converging on the gas, any movement of the atom was expected to cause a force opposing the movement, since the wave facing the atom has an apparent frequency approaching resonance due to the Doppler effect. The result announced by the Bell Labs physicists[4] was sensational:

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[1] Steven Chu, Claude Cohen-Tannoudji and William Phillips received the 1997 Physics Nobel Prize for their works on cooling and trapping of atoms with lasers during these years. See their Nobel conferences:

Chu S. (1998) The manipulation of neutral particles, *Rev. Mod. Phys.* **70** (3), 685–706.

Cohen-Tannoudji C.N. (1998) Manipulating atoms with photons, *Rev. Mod. Phys.* **70** (3), 707–719.

Phillips W.D. (1998) Laser cooling and trapping of neutral atoms, *Rev. Mod. Phys.* **70** (3), 721–741.

[2] Aspect A., Dalibard J., Heidmann A., Salomon C., Cohen-Tannoudji C. (1986) Cooling atoms with stimulated emission, *Phys. Rev. Lett.* **57** (14), 1688–1691.

[3] Notions necessary to understand this introduction can be found in the first chapter of this book.

[4] Chu S., Hollberg L., Bjorkholm J.E., Cable A., Ashkin A. (1985) 3-Dimensional viscous confinement and cooling of atoms by resonance radiation pressure, *Phys. Rev. Lett.* **55** (1), 48–51.

the atoms remained observable at the intersection of the laser beams for almost a second, a time six orders of magnitude longer than usually allowed when observing atoms moving at hundreds of meters per second at room temperature. The measured temperature was claimed compatible with the theoretical prediction of 240 μK, well below that of most existing cryostats. Thus was achieved the first major objective of the teams engaged in this emerging field, Bill Phillips and Hal Metcalf, Jan Hall, Steven Chu and Arthur Ashkin,[5] Dave Pritchard, and Vladilen Letokhov, author of pioneering proposals, but lacking experimental facilities at the end of the Soviet era.

The second major objective was the trapping of neutral atoms. As early as 1985, Bill Phillips' team had succeeded at the magnetic trapping of sodium atoms "stopped" at the end of his Zeeman slower in a minimum of magnetic field.[6] The magnetic trapping method was only valid for paramagnetic atoms, and laser trapping remained a major goal.

An optical molasses is not a trap: the atoms are "stuck" in it by an incredibly intense viscous force (proportional to the velocity with a negative coefficient), but they nevertheless end up diffusing out of the volume where the laser beams focus, as an attractive force towards the center of the trap is lacking. There was a theoretical controversy among theorists about the possibility of a genuine trapping of neutral atoms with light. A famous article by J.P. Gordon and A. Ashkin had asserted the impossibility of achieving this with the resonant radiation pressure force.[7] They had established a theorem for the radiation pressure force called "optical Earnshaw's theorem", equivalent to the impossibility of trapping an electric charge with electrostatic fields, known as Earnshaw's theorem in English speaking countries, and as Gauss theorem in France. Scientists had therefore turned to the other radiative force, the dipole force. It was predicted that dipole force trapping would provide a potential well, *i.e.* an authentic trapping potential around a maximum of the intensity of a red-tuned laser. Unfortunately, calculations also predicted that the inevitable quantum fluctuations of this trapping force, linked to the spontaneous emission of photons, would heat the atoms, which would be rapidly ejected from the potential well. It seemed that there was a no-go theorem for trapping with either force. The most sophisticated solutions were imagined to overcome that apparent impossibility to trap atoms with light, but it is the simplest one which worked, as mentioned in 1983 in a theoretical article by Claude, Jean and Serge Reynaud,[8] and demonstrated experimentally in 1986 by the group of Chu and Ashkin.[9] It was based on a dipole trap alternated with optical molasses. Atoms, which are massive, react

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[5] Nobel laureate 2018 for optical trapping with optical tweezers and their application to biological systems.

[6] Migdall A.L., Prodan J.V., Phillips W.D., Bergeman T.H., Metcalf H.J. (1985) 1st observation of magnetically trapped neutral atoms, *Phys. Rev. Lett.* **54** (24), 2596–2599.

[7] Ashkin A., Gordon J.P. (1983) Stability of radiation-pressure particle traps – an optical Earnshaw's theorem, *Opt. Lett.* **8** (10), 511–513.

[8] Dalibard J., Reynaud S., Cohen-Tannoudji C. (1983) Proposals of stable optical traps for neutral atoms, *Opt. Commun.* **47** (6), 395–399.

[9] Chu S., Bjorkholm J.E., Ashkin A., Cable A. (1986) Experimental observation of optically trapped atoms, *Phys. Rev. Lett.* **57** (3), 314–317.

only to the time average of both the trapping effect of the dipole trap and the cooling effect of optical molasses. Another possibility was found to bypass the optical Earnshaw's theorem, thanks to the internal multilevel structure of the atoms: the celebrated Magneto-Optical Trap, suggested by Jean and demonstrated by Chu and Pritchard.[10]

After the achievement of the two main initial objectives – cooling of atoms to the lowest temperatures ever obtained, trapping of these atoms –, was the game over? Was the subject of cooling and trapping neutral atoms exhausted? In fact, Nature would be generous with those who chose to pursue the subject.

In early 1988, we were alerted by a phone call from Bill Phillips: he had observed some totally unexpected results on the optical molasses he had created at almost the same time as Steve Chu. He was developing, with his team at NIST, new methods to measure the obtained temperature. All these methods converged towards the conclusion that the observed temperature was much lower than the one announced by Chu's team, clearly lower than the one predicted by the simple theoretical model used so far: Phillips' group announced a temperature not exceeding 40 μK[11] instead of Chu's 240 μK, as predicted by the simple theory. Moreover, he had made incomprehensible observations in the framework of the Doppler molasses model: a difference in intensity between two counter-propagating laser beams, which should have led to the rapid loss of atoms under the effect of the non-zero difference in radiation pressures, did not seem to particularly affect the molasses. Christophe and Jean immediately started to investigate the question experimentally, while Claude and Jean took up the theoretical question from every possible point of view in an attempt to understand these surprising and exciting results, contradicting the Murphy's "law" that "if things do not happen as expected, then it's bound to be worse than expected".[12]

The suspicion soon arose that, unlike the two-level atom model used up to that point, "two-level atoms do not exist in the real world, and moreover atoms used in experiments are not one of them" – according to an interesting statement by Bill Phillips, which has remained famous. Indeed, both Bill's sodium atoms and Christophe's and Jean's cesium atoms have a hyperfine structure in the ground state, and this state breaks down into different sublevels whose energies vary according to the intensity and polarization of the light that illuminates them: this results in the famous light shifts studied by Claude in his PhD thesis 30 years earlier. The remarkable Sisyphus model would soon emerge, in which the optical pumping of Kastler and Brossel together with Claude's light shifts combine to force the atom to lose its kinetic energy by constantly climbing up the potential hills of the light displacements; during the climb, rather upwards, the optical pumping would abruptly put them back at the foot of a new hill, associated with another sublevel,

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[10] Raab E.L., Prentiss M., Cable A., Chu S., Pritchard D.E. (1987) Trapping of neutral sodium atoms with radiation pressure, *Phys. Rev. Lett.* **59** (23), 2631–2634.

[11] Lett P.D., Watts R.N., Westbrook C.I., Phillips W.D., Gould P.L., Metcalf H.J. (1988) Observation of atoms laser cooled below the doppler limit, *Phys. Rev. Lett.* **61** (2), 169–172.

[12] Note that this "law" is quite useful when it is considered for security of potentially dangerous installations such as dams or nuclear plants.

without any change in the kinetic energy. The famous ICAP conference (International Conference on Atomic Physics), hosted in Paris in the summer of 1988, endorsed Bill Phillips' experimental results, and Jean and Claude's Sisyphean interpretation,[13] while Steven Chu gave his own interpretation, also based of course on the existence of several sublevels.

Steven Chu had corrected downward his first experimental value, which was wrong for a subtle reason. His first assessment was based on the so-called "release and recapture" method: at the temperature of several hundred microKelvin the atomic velocities were such that if the molasses lasers were turned off for a few milliseconds before being turned back on, the atomic cloud had spread out ballistically, enough for a significant fraction of the atoms to be recaptured. A model based on the Maxwell–Boltzmann distribution allowed calculating the lost fraction which increased with temperature, and it was sufficient to evaluate the temperature corresponding to the observation. But in fact, as understood after Bill Phillips' discovery, at the much lower temperatures of the molasses, the atomic velocities of the released atoms were too low, when the molasses lasers were turned off, to cause a rapid expansion of the cloud: the dominant effect was that of gravity. In a way, the molasses "fell like a stone", which of course led to a loss of atoms during the recapture, but the estimation of the value of this loss by the Maxwell–Boltzmann distribution was totally wrong. And as it happened, by chance, that the obtained value was not very different from the theoretical prediction, one can understand the publication of a wrong result. Let Steven Chu himself draw the lesson of his misadventure in his Nobel lecture: 'Our first measurements showed a temperature of 185 μK, slightly lower than the minimum temperature allowed by the theory of Doppler cooling. We then made the cardinal mistake of experimental physics: instead of listening to Nature, we were overly influenced by theoretical expectations. By including a fudge factor to account for the way atoms filled the molasses region, we were able to bring our measurement into accord with our expectations.' We must be grateful to Steve for the lesson.

The ICAP conference in Paris was the scene for another "coup de theatre" in the field of cooling. After having crossed the Doppler limit, thanks to the Sisyphus effect, one could ask what was the ultimate limit of laser cooling of atoms. One answer seemed obvious: the recoil velocity for a single photon, more precisely the temperature associated with the recoil velocity of an initially stationary atom that absorbs or emits a single photon. A simple reasoning led to this conclusion. It was based on the idea that in order to obtain cooling, a dissipative process is needed, *i.e.*, spontaneous emission, which is the only dissipative process of the atom-radiation interaction. But, the spontaneous emission in free space has a random direction. The final velocity had therefore an average uncertainty related to the "last spontaneous photon emitted" at least equal to the recoil velocity. The associated temperature – called "recoil temperature"– is four orders of magnitude lower than the Doppler "limit" in the case of sodium, *i.e.*, a few tens of nanokelvin, clearly below the Sisyphus limit. Could we reach that ultimate limit?

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[13] Dalibard J., Cohen-Tannoudji C. (1989) Laser cooling below the doppler limit by polarization gradients - simple theoretical models, *J. Opt. Soc. Am. B-Opt. Phy.* **6** (11), 2023–2045.

In fact, in the winter of 1987–1988, at the exact moment when the first information on sub-Doppler temperatures was coming out, Claude and I had envisaged a radically different cooling process, based not on a frictional force that slows down the atoms, but on the "selection" of atoms subject to a Brownian motion and arriving by chance at a zero value of the velocity where they accumulate. In the process we were considering, called "Velocity Selective Coherent Population Trapping" (VSCPT), the velocity of the atoms – again with several fundamental Zeeman sublevels – evolved randomly under the effect of fluorescence cycles resulting from the action of counter-propagating lasers of the same frequency. If the polarizations of the lasers were well chosen, the atoms could fall, by chance, in a superposition state of the Zeeman sublevels which was "dark", not able to absorb any light. The atom would then remain in this state indefinitely, provided that the laser frequencies were strictly equal in the atom's frame of reference, which was only true if the atom was strictly at rest. Otherwise, it would resume its Brownian motion until falling into a dark state with zero speed. Thus, one could hope to accumulate atoms around zero velocity, by a process equivalent to Maxwell's demon. The first time this idea came up, I immediately thought of Raymond Castaing, whose statistical thermodynamics course I had taken at Orsay: he explained that no fundamental law could exclude Maxwell's demon type process, provided that the entropy removed from the cooled sample is transferred to another component of the ensemble. Here, the answer was obviously in relation with the spontaneous photons, totally disordered since they are emitted in any direction.

At that time, we were developing a setup for radiative cooling of metastable helium (He*), with two PhD students, Robin Kaiser and Nathalie Vansteenkiste (now Westbrook), with the help of the metastable helium team at LKB, who was working under the direction of Franck Laloë on quantum statistical effects. Michèle Leduc, a world specialist in lasers at the resonance wavelength of He* at 1.08 μm, as well as Pierre-Jean Nacher and Geneviève Tastevin, constantly helped teaching us how to produce He*. It turned out that the fundamental level of ^{4}He*, with angular momentum $J = 1$, had a sublevel structure perfectly adapted for VSCPT sub-recoil cooling and within a few months our team could demonstrate the one-dimensional effect, just before ICAP. We were able to reach the temperature of 2 μK, below the recoil temperature of 4 μK for metastable helium (this recoil temperature is higher than for alkalis because of the lower mass of helium). The article, submitted on July 11, 1988, was published[14] on August 15, 1988. We had asked Ennio Arimondo to join us. A decade earlier he had contributed to the understanding of coherent population trapping (non-velocity selective) observed by Adriano Gozzini in his laboratory in Pisa. This was the basis of VSCPT cooling.

The study of VSCPT cooling was to continue for several years, on the one hand experimentally with its implementation in two and then three dimensions by François Bardou, who too soon passed away, John Lawall and Michèle Leduc. It also gave rise to a totally unexpected and powerful theoretical analysis that still

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[14] Aspect A., Arimondo E., Kaiser R., Vansteenkiste N., Cohen-Tannoudji C. (1988) Laser cooling below the one-photon recoil energy by velocity-selective coherent population trapping, *Phys. Rev. Lett.* **61** (7), 826–829.

astonishes me, based on a non-standard statistical phenomenon called “Lévy flight”. Such an analysis was born from a meeting of Claude, François and me with Jean-Philippe Bouchaud, with whom we later wrote a book on the subject.[15] Among the most extraordinary predictions of this analysis, the unusual fact that there is no temperature limit: the temperature obtained is predicted to decrease monotonically towards absolute zero when the duration of the interaction of atoms with light increases.

It is in the field of quantum gases, the central subject of the present book, that I will take my third example of a discovery that has benefited from a “favorable nudge” of Nature: the Bose–Einstein condensation of metastable helium. Because of the unique possibility of detecting individual atoms of metastable helium, we decided, with Chris Westbrook, to develop a set up for cold metastable helium atoms in our group of atom optics at the Institut d’Optique, created in Orsay in 1993. Our long term goal was to start a program of quantum atom optics, by analogy with photon quantum optics which developed after the second world war thanks to detection methods of individual photons. This program, still in progress, had started with modest objectives when Antoine Browaeys, a new PhD student, who had taken over the He* set-up at Institut d’Optique from Guillaume Labeyrie, proposed to try to obtain Bose–Einstein condensation of the bosonic isotope ^{4}He*. The bet seemed lost in advance, since the condensation required a phase of evaporative cooling during which the atoms re-thermalize by elastic collision. Indeed, it was well known that two colliding metastable helium atoms de-excite inelastically by so called Penning ionization, releasing a huge energy (on the scale of cold atoms) of several tens of electron volts, more than enough to eject atoms from the cold sample. To this objection, Antoine replied that a Russian theorist, Gora Shlyapnikov, whom we would soon get to know better since he took a position at CNRS, had predicted a suppression of the Penning collision rate by 5 orders of magnitude (a factor of 100 000!) provided that the atoms were polarized, all in the same Zeeman sub-level $m = 1$ of the metastable $2^3\mathrm{S}_1$ state of angular momentum $J = 1$. After many discussions, Antoine convinced Chris, Denis Boiron and myself to let him embark into that project.

I will skip all the novel developments that Antoine had to invent during his thesis, but I will tell how this condensation, the only one yet seen with a metastable noble gas, was produced, with a bit of luck. Antoine had to defend his thesis (brilliant though it was) without having obtained the condensation, for administrative reasons. He then joined Bill Phillips in Gaithersburg. Two new PhD students, Alice Robert and Olivier Sirjean, had taken over the experiment and were pushing as far as they could the evaporative cooling developed by Antoine.[16] But because of the decrease in the number of atoms during the evaporation, they always arrived at a point where the signal became very weak and eventually ceased to be observable. This signal resulted from the observation of the atoms arriving on a detector located

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[15] Bardou F., Bouchaud J.-P., Aspect A., Cohen-Tannoudji C. (2002) *Lévy statistics and laser cooling: how rare events bring atoms to rest.* Cambridge University Press.

[16] Browaeys A., Robert A., Sirjean O., Poupard J., Nowak S., Boiron D., Westbrook C.I., Aspect A. (2001) Thermalization of magnetically trapped metastable helium, *Phys. Rev. A* **64** (3).

five centimeters below the magnetic trap from which they had been released at the end of the cooling phase. The dispersion of the arrival times made it possible to deduce the distribution of the departure velocities, thus to evaluate the temperature, and to verify the efficiency of the cooling. Tired of seeing the signal disappearing when they pushed the evaporation a little too far, the PhD students tried a desperate maneuver: they continued the evaporation despite the disappearance of the signal. And suddenly a signal reappeared, with much cooler atoms, displaying the famous characteristic peak of Bose–Einstein condensation.[17] I do not remember if we immediately thought of the then fifteen years old story of Steven Chu's optical molasses "falling like a stone", but it did not take long for us to understand that a similar phenomenon had occurred in our laboratory: as long as the temperature had not reached a sufficiently low value, the atomic cloud spread rapidly in an isotropic way when the trap was turned off, and only a small fraction of the atoms reached the detector placed five centimeters below the trap. But below ten microkelvin, the initial velocities were so low that all the atoms fell on the detector, resulting in a dramatic increase in the effective detection efficiency. I will not expand on the other favorable element of this experiment, suffered rather than planned, but crucial: because of eddy currents, the magnetic field was submitted to a violent rotation when the magnetic trap was switched off, in a time that we could not reduce to less than a few milliseconds. But in a much shorter time, a fraction of a millisecond, about 10% of the atoms trapped in their $m = 1$ state underwent a non-adiabatic transfer to the $m = 0$ state where they were no longer sensitive to the magnetic field of the trap, even though it was still present, and they fell freely towards the detector. The distribution of arrival times allowed us to reconstruct the distribution of atomic velocities at the time of the trap cut-off, on the one hand, because the fall was not disturbed by the magnetic fields, and on the other hand, because the transfer took place in a short time compared to other characteristic times of the problem.

One week later, the He* team at ENS, around Franck Pereira dos Santos, Michèle Leduc and Claude Cohen-Tannoudji, whom we had immediately informed of our success, observed the phenomenon of condensation of metastable helium with a different method.[18] Since then, we have been able to develop as planned our program of quantum atomic optics,[19] which is still in progress, while David Clément has developed another He* experiment for a unique quantum simulator of condensed matter phenomena.[20]

I could have cited other examples of remarkable and unexpected discoveries, contradicting some "impossibility theorems", which have peppered the experimental

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[17] Robert A., Sirjean O., Browaeys A., Poupard J., Nowak S., Boiron D., Westbrook C.I., Aspect A. (2001) A Bose–Einstein condensate of metastable atoms, *Sci.* **292** (5516), 461–464.

[18] Dos Santos F.P., Leonard J., Wang J.M., Barrelet C.J., Perales F., Rasel E., Unnikrishnan C.S., Leduc M., Cohen-Tannoudji C. (2001) Bose–Einstein condensation of metastable helium, *Phys. Rev. Lett.* **86** (16), 3459–3462.

[19] Aspect A. (2019) Hanbury Brown and Twiss, Hong Ou and Mandel effects and other landmarks in quantum optics: from photons to atoms, in Current Trends in Atomic Physics. Oxford University Press. Manuscript available at https://arxiv.org/abs/2005.08239.

[20] Carcy C., Cayla H., Tenart A., Aspect A., Mancini M., Clement D. (2019) Momentum-space atom correlations in a Mott insulator, *Phys. Rev.* X **9** (4).

progress in the field of ultra-cold quantum gases. But it is time to conclude this preface, by drawing some lessons from sometimes surprising trajectories of experimental physics. First, as shown from the episodes of Steven Chu's optical molasses and the observation of metastable helium condensation, one should not think that what one observes in a real experiment is systematically a degraded version of what was predicted. Nature is always more complex than our simple models, and even if it is true that this complexity is often the cause of less spectacular results than expected, it also leaves open the possibility of subtle phenomena not anticipated, like the Sisyphus effect, leading to better results than expected: an anti-Murphy's law!

I want to add a word about the proper use of impossibility theorems — I am of course talking about exact theorems, not theorems with mistakes. It is important to understand what the conditions for the application of the theorem are; then, if all these conditions are not met, it may be possible to pass the limits set by the theorem. We know the case of trapping of charged particles, considered impossible according to the Earnshaw–Gauss theorem, which in fact applies only to electrostatic fields, but neither to Penning traps nor to Paul traps, which use alternating magnetic and electric fields. I have mentioned the case of the magneto-optical trap which escapes the optical Earnshaw's theorem by not respecting the proportionality relation between the Poynting vector and the radiation pressure, again because of the multilevel structure of real atoms. I have also shown how the recoil limit, associated with cooling processes resulting from a frictional force, has been beaten by a process that is not a dissipative process in the usual sense of the term, since the atoms are cooled not by a frictional force but by a selective accumulation in velocity space.

Far from being a science of the past, as it was sometimes considered, the physics of atoms interacting with light, at the origin of the development of quantum physics at the beginning of the 20th century, experienced an extraordinary revival with the cooling of atoms by laser, followed by the study of ultra-cold quantum gasses thus created. In AMO physics, we have a priori exact theoretical descriptions, but we must develop simplified models to solve the sometimes inextricable equations and to obtain simple images giving fruitful intuitions. It is the confrontation of these simplified models with experimental observations that can give rise to the happy surprises of which I have given some examples. There is no doubt that new and equally extraordinary surprises can be expected by the researchers. It will be exciting to follow these new developments, to which the reading of this book will have prepared the reader.

Palaiseau and Oléron, June 2020

Contents

CHAPTER 5

CHAPTER 6

CHAPTER 7

CHAPTER 8

Chapter 1

Cooling and Trapping Atoms

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[2]Emeritus Research Director at CNRS, Laboratoire Kastler Brossel, Paris

This chapter introduces the main methods developed over the last decades to cool and trap ensembles of atoms at extremely low temperatures, down to a billionth of a degree above the absolute zero. These methods are essentially based on the interaction of atoms with light. Here, we present the two greatest advances in the field, laser cooling and trapping in the 1980s, followed by the achievement of Bose–Einstein condensation in 1995, which earned the actors of these discoveries the Nobel Prize in Physics in 1997 and 2001. Since then, the range of methods for manipulating atoms has grown considerably; a wide variety of traps have been created. The extension to fermions of the methods initially developed for bosons has further enriched these perspectives. Cold atom gases have thus become extremely well controlled systems, offering many possibilities of research in various fields of physics.

1.1 When an Atom Meets a Photon

An atom can be described by a set of energy levels corresponding to the different possible quantum states in which it can be found. To account for this set of energy levels (or spectrum), Niels Bohr introduced in 1913 a planetary model of the atom in which the electrons revolve around the nucleus: the faster the electron spins and the further away from the nucleus, the higher is the electron energy. In the case of the hydrogen atom, the electron (of negative charge) revolves around the nucleus made

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up of a proton (of positive charge). Niels Bohr postulates that only certain trajectories are possible, each one associated with a different energy level[1].

This structure in energy levels is very complex, but in some cases, it can be reduced to a two level system, with a lower energy level called the fundamental level and a higher energy level called the excited level. This is the model that we will adopt in the following. For the atom to pass from its fundamental level to the excited level, it must be supplied with an energy equal to the energy difference E between the two levels, which can be linked to a frequency *via* the Planck constant h according to $E = h\nu_0$. This energy is supplied by light *via* the absorption by the atom of a grain of light or photon (see figure 1.1): only photons of frequency ν_0 will allow the atom to change level. Once the atom is placed in the excited level, it will, after a certain time, de-excite and return to its fundamental level by emitting a photon of energy equal to the difference in energy between its two levels. This process is called spontaneous emission. Thus light and matter exchange energy by "packet" of energy or quantum of energy, hence the term quantum physics.

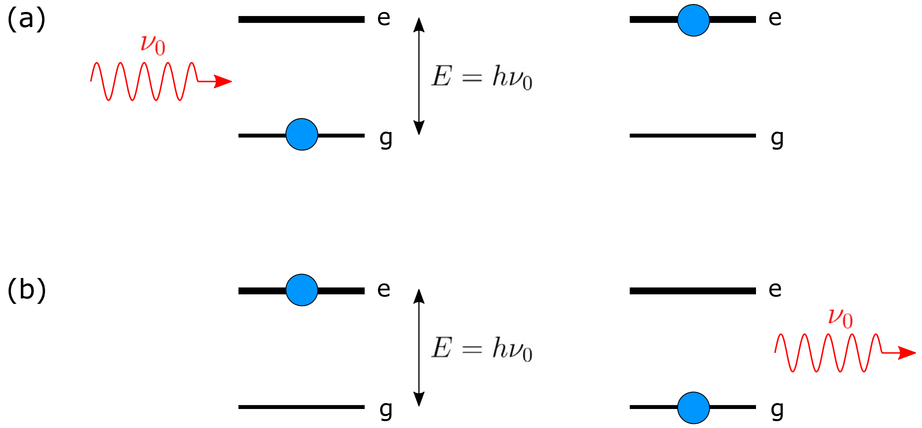

Fig. 1.1 – (a) The atom initially in its ground state (level g) absorbs a photon of energy $h\nu_0$ (with ν_0 the frequency of the electromagnetic wave associated with the photon) equal to the energy difference E between the fundamental level and the excited level (level e). After absorption, the atom is in the excited state. (b) The atom de-excites by spontaneous emission of a photon of energy $h\nu_0 = E$.

During the absorption or emission of a photon by the atom, energy is conserved: in the case of absorption, the initial state corresponds to an atom in its ground state and a photon of energy $h\nu_0$; the final state corresponds to an atom in its excited state (its energy is then increased by the quantity $E = h\nu_0$) and the photon has

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[1] One should note that if this Bohr model allows understanding the idea of energy levels, it was subsequently refuted by experimental observations.

disappeared. Processes of absorption and spontaneous emission are also accompanied by a transfer of momentum between the atom and the photon. The momentum of an atom is the product of its mass m by its speed v and that of the photon is defined by h/λ_0 where $\lambda_0 = c/\nu_0$ is the wavelength associated with the photon with c the speed of light. Thus the phenomena of absorption and spontaneous emission modify the velocity of the atom and will therefore be used to slow and cool down an ensemble of atoms.

1.1.1 The Atom Slows Down...

To slow down an atom beam, we use a laser beam propagating in the direction opposite to the velocity of the atoms. When the laser frequency is well chosen (we will come back to this point in the following), an atom of velocity v absorbs a photon. The atom is then in its excited state, and the momentum of the atom decreases by an amount exactly equal to the momentum of the photon. Before absorption, the atom had a momentum equal to mv and the photon a momentum equal to h/λ_L with λ_L the wavelength of the laser. As the atom and the laser propagate in opposite directions, the momentum of the atom after absorbing the photon is therefore $mv - h/\lambda_L$.

After a while, the atom de-excites and emits a photon in a random direction. The atom can then absorb another photon and make another cycle (see figure 1.2). In fact the atom undergoes a large number of absorption-spontaneous emission cycles and on average, only the absorption steps modify the momentum of the atom, proportionally to the momentum of a photon multiplied by the number of cycles. We can understand this process in terms of force: the atom undergoes an average force exerted by the laser, called the radiation pressure force. This process is very efficient: typically it is possible to stop the propagation of an atomic beam of velocity equal to 300 m/s over one meter. This corresponds to a deceleration several thousand times greater than the acceleration of gravity.

In fact, the laser beam used for slowing down is not exactly resonant with the atomic transition: we say that the laser is detuned from the transition. We choose a laser beam with a frequency slightly lower than the frequency ν_0 of the transition, which corresponds to a laser wavelength slightly higher than the wavelength associated with the atomic transition. Why do we shift the frequency of the laser beam involved in the slowing down? To understand this, one has to take into account the Doppler effect, which makes, for example, that we hear the siren of a fire truck differently when it comes towards us or moves away from us. Let us consider two frames: the laboratory frame in which the atom moves at velocity v in a direction opposite to the direction of propagation of the laser of frequency ν_L; and the frame of the atom in which it is at rest. In the atom frame, due to the Doppler effect, the laser frequency felt by the atom is increased compared to ν_L by a quantity v/λ_L with λ_L the laser wavelength; thus the laser is felt by the atom as

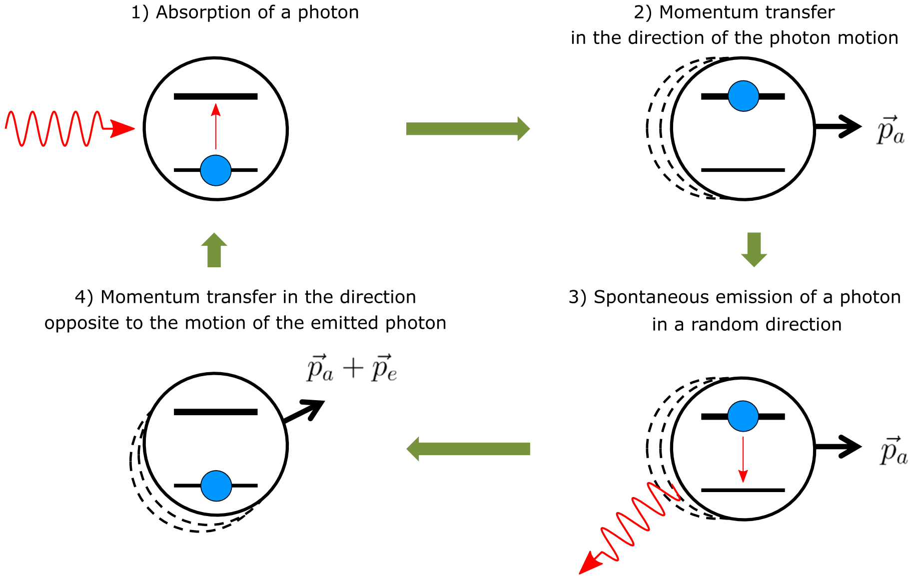

FIG. 1.2 – Momentum transfer: an atom initially in its ground state absorbs a photon resonant with its transition and undergoes momentum transfer $\vec{p}_a$ in the direction of the photon. By spontaneous emission, it de-excites by emitting a photon in a random direction, which transfers momentum $\vec{p}_e$ to the atom. Once again in its initial state, the atom is ready to start a new cycle by absorbing a new photon. By averaging this effect over a large number of cycles, the momentum acquired by the atom during the spontaneous emission stages is canceled out while the one acquired during the absorption stages is similar to a pressure force in the direction of the incident photon.

being closer to resonance. The probability that the atom will absorb a photon from the laser beam is then increased. On the contrary, in the case where in the laboratory frame, the atom and the laser beam propagate in the same direction, the frequency seen by the atom in its frame is lower than the frequency chosen by the user ν_L.

Let us go back to the slowing down of an atom beam. The higher is the velocity of the atoms, the higher is the frequency shift due to the Doppler effect. Thus the frequency shift decreases during the slowing down of the atoms. In order to maintain an efficient deceleration regardless of the velocity of the atoms, the frequency of the atomic transition ν_0 can be changed using a magnetic field in order to keep the laser resonant with the atomic transition; this is the principle of the Zeeman slower (see figure 1.3).

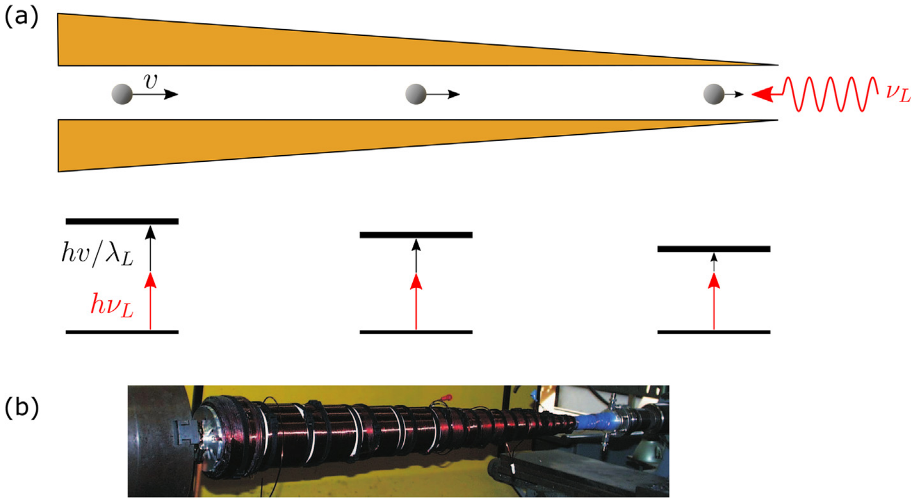

FIG. 1.3 – (a) Principle of a Zeeman slower: in the laboratory frame, an atom of velocity v is illuminated by a laser beam, propagating in the opposite direction, of frequency v_L detuned with respect to the atomic transition frequency. Let us consider that the atom has a velocity such that in the atom frame, it sees the laser beam at resonance. When the atom velocity decreases under the effect of the slowing down, the atom thus no longer sees the laser at resonance and cannot be slowed down effectively. We therefore add an inhomogeneous magnetic field created by a coil (here shown in yellow) so as to modify the atomic transition frequency in order to exactly compensate for the variation of the atom velocity. The atom thus sees the laser at resonance regardless of its velocity and can be effectively slowed down. (b) Photograph of the winding of a Zeeman slower used to slow down chromium atoms. Photograph taken from Arnaud Pouderous' thesis, University Paris 13 (2007). Design and production at the mechanical workshop of the Laboratoire de physique des lasers, CNRS and Paris 13 University (UMR 7538) by Etienne Maréchal and René Barbé.

1.1.2 ... The Gas Temperature Drops

Until then we have considered the slowing down of an atom beam, *i.e.* the decrease in the average speed of the atoms. Now if we want to cool a cloud of atoms, we have to reduce its velocity dispersion, *i.e.* the deviations of the atom velocities compared to the average velocity. Let us consider a gas of atoms whose average velocity is zero and suppose for the moment that the atom velocities are all oriented along an axis, in one direction or the other. To cool the gas, we will illuminate it with two laser beams of the same frequency v_L, propagating in opposite directions (see figure 1.4). The frequency of the laser beams is always chosen to be slightly lower than the atomic transition frequency. An atom propagating at velocity v along the laser axis will preferentially interact with the laser propagating in the opposite direction: in the atom frame, this laser is seen with a frequency $v_L + v/\lambda_L$ closer to resonance while the other laser is seen with a frequency $v_L - v/\lambda_L$ further from resonance. The radiation pressure forces exerted by the two lasers are imbalanced and the resulting force experienced by the atom is then a frictional force which opposes the atom velocity.

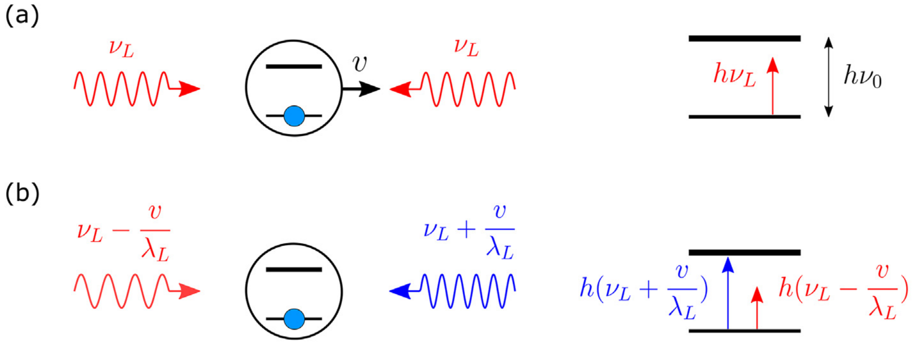

FIG. 1.4 – (a) In the laboratory frame, an atom of velocity v is illuminated by two laser beams, of frequency ν_L detuned from the atomic transition frequency ν_0, propagating in opposite directions. (b) In the atom frame, the atom is at rest and sees the laser beams shifted in frequency due to the Doppler effect: the beam propagating in the opposite direction with respect of the atom velocity in the laboratory frame is seen with a higher frequency $\nu_L + v/\lambda_L$ and therefore closer to resonance. The other beam is seen by the atom with a lower frequency $\nu_L - v/\lambda_L$ and therefore further away from resonance.

In reality atoms can move in any direction in space. To cool the cloud of atoms along the three axes, one illuminates the cloud with three pairs of laser beams, the two beams constituting a pair propagating in opposite directions. The configuration of the laser beams is shown in figure 1.7. This is referred to as optical molasses, in which the atoms are "stuck". Laser cooling and trapping of atoms was crowned by the 1997 Nobel Prize in Physics, awarded to S. Chu (Stanford, USA), C. Cohen-Tannoudji (ENS Paris) and W. Phillips (NIST, USA) (see figure 1.5).

FIG. 1.5 – S. Chu (Stanford University, USA), C. Cohen-Tannoudji (Collège de France, CNRS and ENS Paris, France) and W. Phillips (NIST, USA) received the Nobel Prize in Physics in 1997 "for development of methods to cool and trap atoms with laser light".

1.2 Atomic Traps of All Kinds

So far we have been interested in the laser cooling of an atomic cloud. To be able to carry out these cooling experiments, it is essential to decouple the atoms from their environment: the atoms that we are trying to cool should not be in contact with surfaces or collide with atmospheric molecules. This would annihilate all efforts made to cool the atomic cloud. This implies to carry out cooling experiments in setups in which a very high vacuum is established and also being able to trap and manipulate the atoms far from the walls of the vacuum system, which are at room temperature (see figure 1.6).

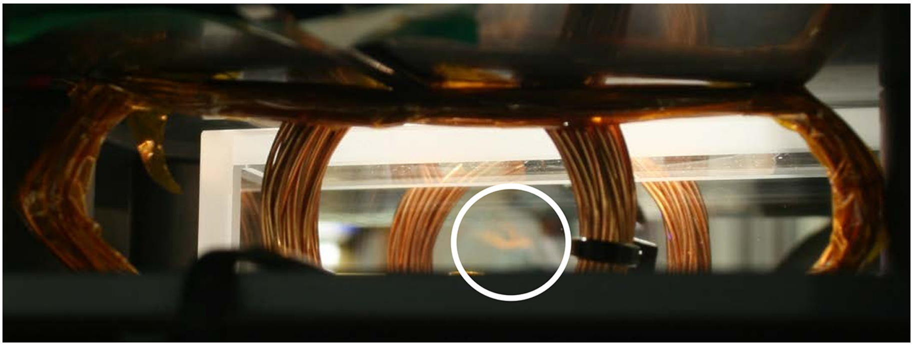

FIG. 1.6 – Photograph of an experimental cold atom setup: a cloud of atoms cooled by laser (in orange) is trapped at the center of a glass cell under vacuum, surrounded by magnetic field coils (Laboratoire Collisions Agrégats Réactivité, Toulouse).

In this section, we will focus on the different traps used with cold atoms. In general, these traps are based either on the use of laser beams or on the use of magnetic fields, but it is also possible to combine both optical and magnetic trapping.

1.2.1 With Lasers and a Magnetic Field: The All-Purpose Trap

As we have seen, the frictional force at work in optical molasses is independent of the position of the atoms. To make this process dependent on the position and thus to trap and cool the atoms at the same time, we introduce an inhomogeneous magnetic field. This first trap, called magneto-optical trap, is an essential step when trying to trap and cool atoms.

In practice, the magnetic field is obtained using two identical coils placed symetrically with respect to the point where all laser beams intersect, fed with opposite currents (see figure 1.7). The magnetic field is then zero at the center and

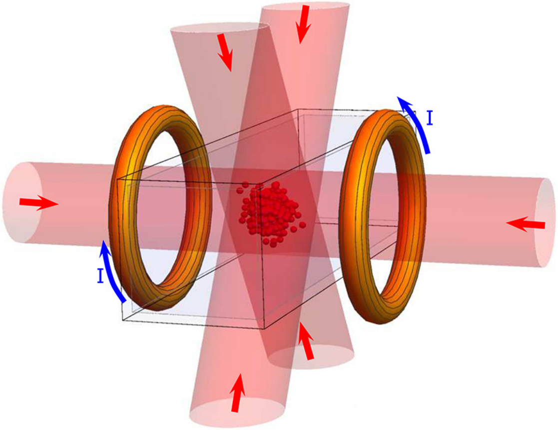

Fig. 1.7 – Schematic diagram of a magneto-optical trap: the atoms are trapped and cooled by the trap combining three pairs of laser beams propagating two by two in opposite directions and an inhomogeneous magnetic field obtained by circulating currents in opposite directions in two identical coils (Cold Atoms team, Laboratoire Collisions Agrégats Réactivité, Toulouse).

increases as a function of the distance from the trap center. It is also necessary to pay attention to the polarization of the laser beams. The polarization of an electromagnetic wave corresponds to the evolution of the direction of the electric field vector during its propagation. In the case of the magneto-optical trap, the beams, propagating two by two in opposite directions, have circular polarizations: this means that in a plane perpendicular to the direction of propagation, the extremity of the electric field vector describes a circle over time. The directions of travel on the circle are opposite for each beam.

Let us consider in the following a single pair of laser beams and an inhomogeneous magnetic field along the direction of propagation of the beams. The inhomogeneous magnetic field allows, as in the case of the Zeeman slower, to tune the energy levels of atoms according to their position with respect to the trap center and therefore to modify the resonance frequency according to the position of the atoms. Taking into account the polarizations of the laser beams, the radiation pressure forces induced by the two laser beams acting on an atom that is not in the center are imbalanced. This results in a restoring force which tends to bring the atoms back to the trap center and allows to trap them (see figure 1.8).

This magneto-optical trap is said to be dissipative in the sense that the trap dissipates energy and thus cools the cloud of atoms. This cooling is so efficient that the atoms collected by this trap (typically one billion in a volume on the order of 1 cm^3) pass from room temperature (around 300 K) to a few hundred microkelvins, *i.e.* a decrease of six orders of magnitude, in a fraction of a second. To explain the Doppler cooling process, we only considered the average effect of a large number of absorption-spontaneous emission cycles. We thus considered that on average the spontaneous emission steps did not lead to any modification of the atom

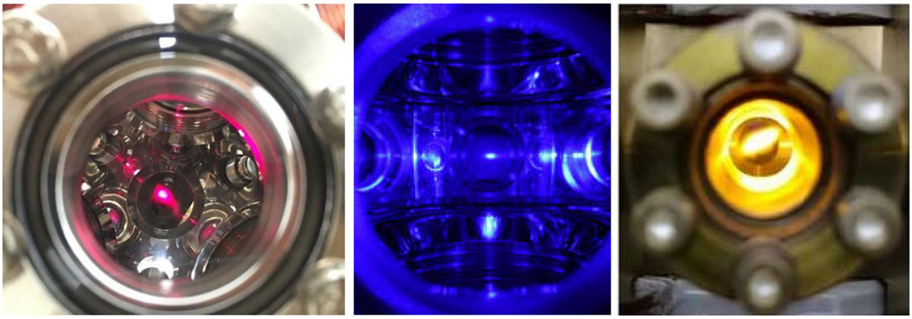

Fig. 1.8 – Magneto-optical traps for lithium atoms (Fermi gas team, Ecole normale supérieure, Paris), strontium (Marc Cheneau's team at Institut d'Optique, Palaiseau), and sodium (credit: Dany Ben Ali, Laboratoire de physique des lasers, Villetaneuse). After absorption of the light coming from the lasers used for cooling, the trapped atoms re-emit light by spontaneous emission, which allows to detect them. The wavelength of the light emitted by spontaneous emission is specific to the atomic species: 671 nm for lithium, 461 nm for strontium and 589 nm for sodium. Thus each cloud of atoms, here at the center of each photo, shines with a different color.

momentum. However, at the end of each spontaneous emission step, the momentum of the atom is modified. These successive random variations in the atom momentum cause the atomic cloud to heat up, which ultimately limits the temperature of the cloud. Let us note that experimentally, the measured temperatures are lower than those expected, because more complex processes, known as sub-Doppler cooling, also come into play.

However, the minimum temperature remains limited in this type of trap. Decreasing the temperature of the atomic cloud further requires the use of another type of traps: the so-called conservative trap, which allows confining a cloud of atoms for very long periods of time, up to several minutes, without additional heating. These conservative traps can be either optical or magnetic, as we will see below, or a combination of the two.

1.2.2 Optical Tweezers to Catch and Immobilize Atoms

To trap atoms, we can use optical traps called optical tweezers. There were invented in the 1980s by Arthur Ashkin, who was awarded the 2018 Nobel Prize in Physics for this discovery. They allow trapping and manipulating all kinds of objects and have, for example, given rise to numerous applications in biology. They use very focused laser beams, the objects being trapped at the point of maximum light intensity (at the point of focus).

The trapping of atoms corresponds to the case where the trapped particle has a very small size compared to the wavelength of the laser used. It relies on the dipolar force which is one of the forces exerted by light on atoms, the other force being the radiation pressure force which is used to cool the atoms. The dipolar force tends to attract atoms towards maxima or minima of light intensity.

To understand the effect of the dipolar force on atoms, we need to introduce the notion of electric dipole. Let us consider the case of a hydrogen atom; it is composed of two particles of opposite charges: a proton and an electron. Under the action of the electric field associated with the light wave, the proton and the electron will undergo opposite forces which push them away from each other. The atom becomes polarized: it acquires an electric moment induced by the electric field and then behaves like a small dipole. This dipole will tend to orient itself in the direction of the electric field: in the case of an inhomogeneous field, it will undergo a force which will attract it towards areas of high laser intensity or repel it from these areas. If the laser is red-detuned, *i.e.* with a wavelength higher than the atomic transition wavelength, the atoms will accumulate in areas of high intensity (see figure 1.9a). To trap the atoms, it is then sufficient to focus a red-detuned laser beam with a lens; the atoms are then trapped at the beam focal point where the intensity is maximum. If the laser wavelength is smaller than the atomic transition wavelength, atoms are repelled by areas of high intensity (see figure 1.9b). In this case, it is generally necessary to combine several laser beams to trap the atoms.

In order to keep the atoms as long as possible in the trap, the radiation pressure force resulting from the absorption of photons should be negligible. This implies using far-off resonance lasers. If one seeks for example to achieve a trap with a single laser beam, one will generally use lasers with wavelengths in the infrared, for instance in the range of wavelengths used for optical telecommunications (around 1500 nm).

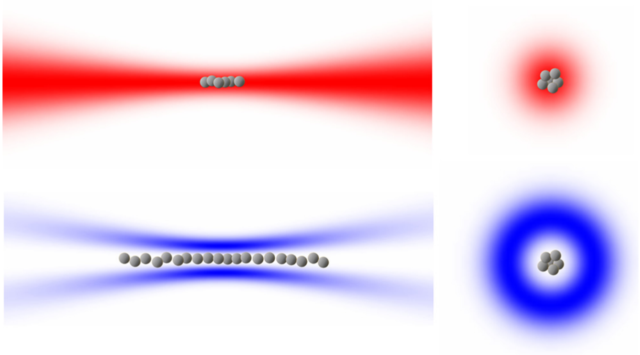

Fig. 1.9 – (Above) Optical dipole trap created by a focused red-detuned laser beam. Atoms accumulate around the maximum intensity. (Bottom) Optical dipole trap created by a blue-detuned beam. The beam has a minimum of intensity at the center towards which the atoms are repelled. However, there is no trapping along the axis of propagation of the light; the cloud can extend freely along this axis.

Optical traps have the advantage of being easy to use and flexible. The geometry of the trap depends directly on the spatial profile of the used laser beam at its focal point. To obtain a trap of smaller size, one just has to focus the laser on a volume of smaller size. By combining several laser beams and by adjusting their power, their size at the point of focus or their polarization, it is possible to create traps with various geometries. When using a single focused laser beam, the created trap is more elongated in the direction of propagation of the beam (longitudinal direction) than in the perpendicular directions (transverse directions). By crossing two laser beams of the same wavelength, we create more isotropic traps, *i.e.* having similar dimensions in the three directions of space (see figure 1.10). We will see below that this last trap is particularly suitable for cooling clouds of atoms to even lower temperatures. It should also be noted that to optically trap a cloud of atoms, the depth of the trap must be greater than the energy $k_B T$ associated with cloud temperature T, with k_B Boltzmann's constant. This implies pre-cooling the cloud in a magneto-optical trap and using lasers with a power of the order of several watts.

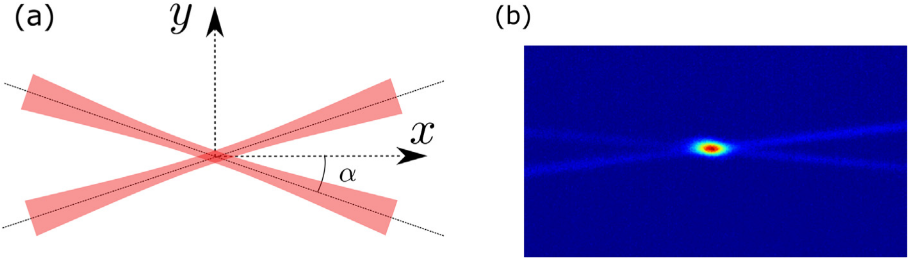

Fig. 1.10 – Trapping of atoms in two crossed laser beams. (a) By crossing two focused beams, it is possible to create a three-dimensional trap for already cooled atoms. (b) Fluorescence image of a set of 20 million rubidium-87 atoms at 30 μK trapped at the crossing of two laser beams at 1070 nm with a power of 20 W (Atom Interferometry team, Laboratoire Collisions Agrégats Réactivité, Toulouse).

1.2.3 With Magnetic Fields: From Large Volume Traps to Atomic Chips

It is also possible to create purely magnetic traps. These are based on the magnetic properties of atoms, which behave like small magnets, characterized by their magnetic moment. We then speak of magnetic dipoles. In the presence of a static magnetic field, the magnetic dipoles will orient themselves along the magnetic field axis: either in the same direction as the field or in the opposite direction. If the field is not uniform, the dipoles aligned in the same direction as the field will be attracted towards the areas of strong magnetic field, the others will be attracted towards the minima of magnetic field. The laws of electromagnetism only allows achieving minima of static magnetic field intensity. It is therefore not possible to trap atoms in any state: we can only trap atoms placed in a state for which their magnetic moment is aligned along the magnetic field axis but in the opposite direction with respect to the field.

The first traps that were developed are so-called macroscopic traps, obtained using a combination of magnetic field coils. The simplest magnetic trap is obtained using two coils with the same axis traversed by currents in opposite directions, in the same way as for the magneto-optical trap (see figure 1.11). The obtained magnetic field, called quadrupolar, exhibits a zero which induces atomic losses: an atom which moves close to the zero can see its magnetic moment flip with respect to the magnetic field. The atom is then no longer trapped and is expelled from the trap. These atomic losses linked to the presence of a zero in the magnetic field, called Majorana losses, increase with the density of the cloud and also induce a deleterious heating when one seeks to cool the cloud of atoms. To avoid these losses, different methods have been developed: one can use static magnetic fields which do not have a zero using more complex coil arrangements; one can also combine a static magnetic trap with a magnetic trap which varies rapidly over time and whose center is offset from that of the static trap: the atoms cannot follow the rapid variations of the magnetic field and see an average magnetic field exhibiting a non-zero minimum; one can also combine the static magnetic trap with a blue-detuned laser so that the atoms cannot reach the zero of the magnetic field: in this last case one speaks of an “optical plug”. The last two configurations were used, respectively, by the groups of E. Cornell and W. Ketterle to obtain the first condensates in 1995. These macroscopic traps use magnetic field coils placed around the vacuum chamber in which the atoms are located. The fields necessary to trap atoms then require strong currents on the order of several tens to several hundreds amperes.

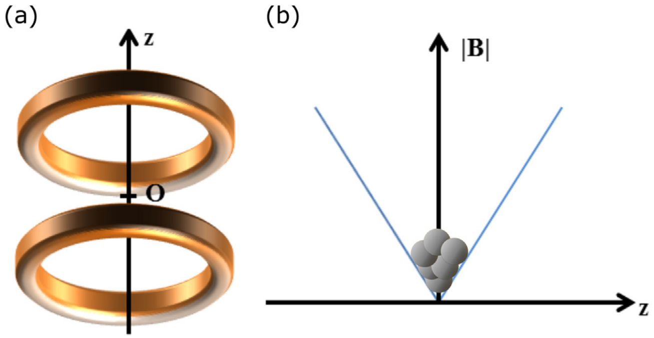

Fig. 1.11 – Magnetic trap: (a) Two identical magnetic field coils traversed by currents of equal intensity flowing in opposite directions create a trap for atoms whose magnetic moment is anti-aligned with the magnetic field. (b) Modulus of the magnetic field along the axis of the coils, the field zero is obtained at the center of symmetry O of the device.

From the perspective of various applications requiring devices of reduced size, for example the production of on-board atomic sensors, efforts have been and are still being made to miniaturize the experimental devices. In this context, miniature magnetic trapping devices, called atom chips, have been developed. An atom chip is a support, placed directly in the vacuum chamber, on which conductive wires of micrometric size are deposited or etched (see figure 1.12a). By circulating a current of a few amperes in the wires and in the presence of a homogeneous magnetic field (see figure 1.12b), it is possible to trap a cloud of cold atoms at a small distance from the surface of the chip, from a few tens of micrometers to a few millimeters. Different geometries of the magnetic trap can be envisaged depending on the arrangement of the different wires on the chip and the current flowing in each of the wires.

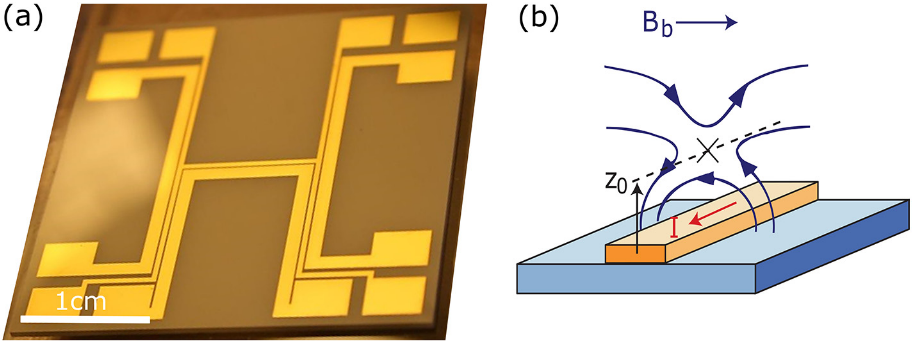

Fig. 1.12 – (a) Atoms chip used in a cold atom experiment (Atom Interferometry team, Laboratoire Collisions Agrégats Réactivité, Toulouse). (b) The flow of current I in the surface wires close to the atoms creates a magnetic field rotating around the wire. The addition of a homogeneous magnetic field B_b perpendicular to the wire cancels the field created by the chip at a certain distance z_0 from the surface thus creating a trap for the atoms in the states attracted by the field minima. Illustration taken from Philipp Treutlein's PhD thesis, University of Munich, Germany (2008).

The advantage of atom chips is that they produce strong magnetic field gradients with modest currents and create very confining traps. It is then possible to drastically increase the collisions between atoms and therefore to obtain condensates very quickly by evaporative cooling, as we will see below. The atomic chips can also be used in combination with macroscopic magnetic traps or with optical traps in order to increase the number of atoms in the obtained ultracold atom cloud. It is also possible to add additional elements on the chip, such as a mirror or an optical guide, for a greater miniaturization of the experimental devices.

1.3 Even Colder: The Gas Changes State

1.3.1 Last Step Towards the Absolute Zero: We Evaporate

Once the atoms are confined in a conservative trap (optical and/or magnetic), there is a final cooling step before obtaining a Bose–Einstein condensate, called evaporative cooling. This step is nothing else than what we do when eating a soup that is too hot: we start by blowing on the soup; it consists physically in eliminating the most energetic particles. The remaining liquid then thermalizes at a lower temperature under the effect of collisions between the constituents of the soup. If the soup has cooled sufficiently, then it can be eaten. If this is not the case, we will blow again on the soup until an acceptable temperature is obtained.

Experimentally, we apply the same principle to cool the atoms. Depending on the type of trap in which the atoms are confined, the techniques for removing the most energetic atoms are different: in the case of an optical trap, the most energetic atoms are allowed to escape from the trap by gradually lowering the power of the focused laser beam creating the trap (see figure 1.13). In the case of a magnetic trap, we use the fact that we cannot magnetically trap atoms in any quantum state. We apply a radio-frequency wave or microwave to transfer the most energetic atoms to a state in which they cannot be trapped; the atoms are then expelled from the trap. The frequency of the radio-frequency wave or microwave, which determines the energy of the expelled atoms, is gradually changed to cool the atomic cloud.

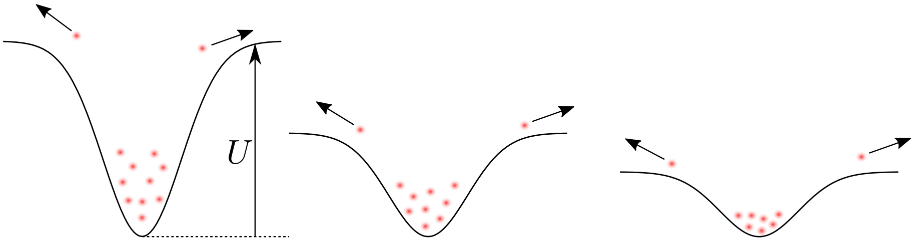

Fig. 1.13 – Principle of evaporative cooling. Atoms are initially confined in a trap of finite depth U. By regularly reducing the depth, the most energetic atoms will escape from the trap and the remaining atoms will thermalize, by collisions, at a lower temperature. In the case of an optical trap, shown here, the reduction in depth is accompanied by a reduction in the stiffness of the trap and therefore of the confinement, which tends to slow down the rethermalization and therefore to make the cooling less efficient.

At the same time, collisions between atoms within the atomic cloud lead to a redistribution of energy and the thermalization of the cloud at a lower temperature. There are two types of collisions: elastic collisions on which evaporative cooling relies on and inelastic collisions which one seeks to minimize. If we consider two atoms that collide, the energy being conserved during this collision, one atom can absorb most of the energy involved in the collision and the other will then have a lower energy. The first atom will be expelled from the trap, the second will remain in the trap (see figure 1.14). Thus for an efficient evaporative cooling process, it is necessary to have the highest possible collision rate and therefore the most confining trap possible. This method of evaporative cooling is efficient, it allows reaching temperatures of the order of a few tens of nanokelvins, at the expense of loosing atoms, generally 999 per 1000.

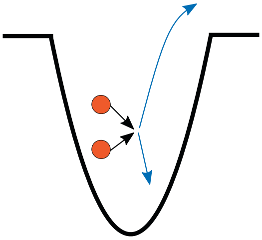

FIG. 1.14 – Principle of thermalization: following a collision, one of the atoms receives most of the energy and can then escape from the trap; the other atom, which has a much lower energy, remains in the trap.

1.3.2 Finally, the Grail, the Bose–Einstein Condensation: The Atoms All as One!

At these very low temperatures, atoms, if they are bosons (see below), undergo a quantum phase transition called Bose–Einstein condensation. This phase transition was predicted by Albert Einstein, based on the work of an Indian physicist Satyendranath Bose. Below a certain temperature called critical temperature T_c, atoms accumulate in the same quantum state. For trapped atoms, the atoms will accumulate in the lowest energy state of the trap (see figure 1.15). This condensation phenomenon is not due to a simple effect of lowering the temperature: at the critical temperature, the thermal energy of the cloud $k_B T$ is still much higher than the difference in energy between two levels in the trap. It is a phenomenon that results directly from the quantum properties of bosons at very low temperatures.

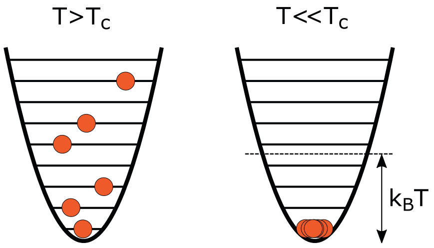

FIG. 1.15 – Bose–Einstein condensation: for a temperature above critical temperature T_c, the bosons are distributed over the different energy states of the trap. When the temperature drops below T_c, bosons accumulate in the lowest energy state. Atoms in this state form a giant matter wave called the Bose–Einstein condensate.

To get an idea of the temperature at which this transition occurs, we need to consider both the particle and wave nature of atoms (see figure 1.16). At high temperatures, the atoms of the gas can be considered as independant point particles: they behave like small balls, the typical distance between atoms being directly related to their density in the cloud. At low temperatures, the same atoms behave like waves whose characteristic extension is given by a length called thermal de Broglie wavelength λ_{dB} which increases when the temperature decreases according to $\lambda_{dB} = \sqrt{h^2/(2\pi m k_B T)}$. The phenomenon of Bose–Einstein condensation appears when λ_{dB} becomes of the order of the typical distance between atoms, that is to say when the waves begin to overlap in the gas. The atoms then gradually accumulate in the lowest energy state of the trap. All atoms in this state behave the same way and form a giant matter wave.

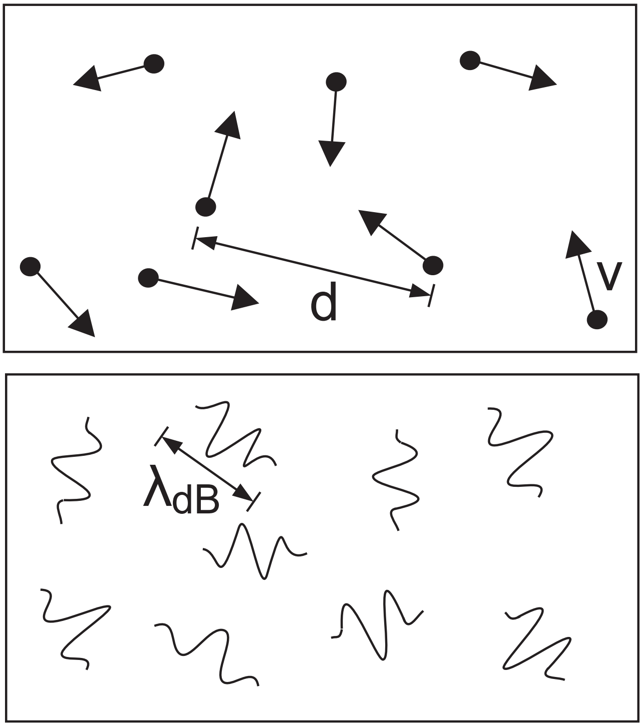

Fig. 1.16 – Criterion for the Bose–Einstein condensation: the condensation appears when the extension of the waves associated with the atoms λ_{dB} becomes on the order of the typical distance d between atoms. Figure taken from W. Ketterle, D. S. Durfee, and D. M. Stamper-Kurn, Making, probing and understanding Bose–Einstein condensates, In Bose–Einstein condensation in atomic gases, Proceedings of the International School of Physics "Enrico Fermi", Course CXL, edited by M. Inguscio, S. Stringari and C. E. Wieman (IOS Press, Amsterdam, 1999).

The first Bose–Einstein condensates were obtained experimentally in 1995 in the groups of E. Cornell and C. Wieman (JILA, USA) and W. Ketterle (MIT, USA), who have been awarded the 2001 Nobel Prize in Physics (see figure 1.17). The condensation transition is observed experimentally from the velocity distribution of the atomic cloud (see figure 1.18): above the critical temperature, the velocity distribution of atoms is Gaussian. Close to the critical temperature, we observe the superposition of the two distributions: one, very narrow, corresponding to the condensate and the other, Gaussian, corresponding to the non-condensed atoms.

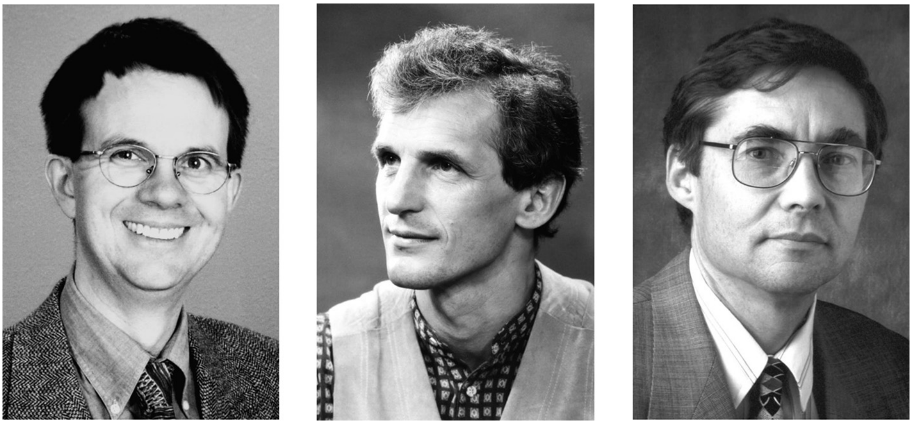

Fig. 1.17 – E. Cornell (JILA and NIST, USA), W. Ketterle (MIT, USA) and C. Wieman (JILA and University of Colorado, USA) received the Nobel Prize in Physics in 2001 “for the achievement of Bose–Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates”.

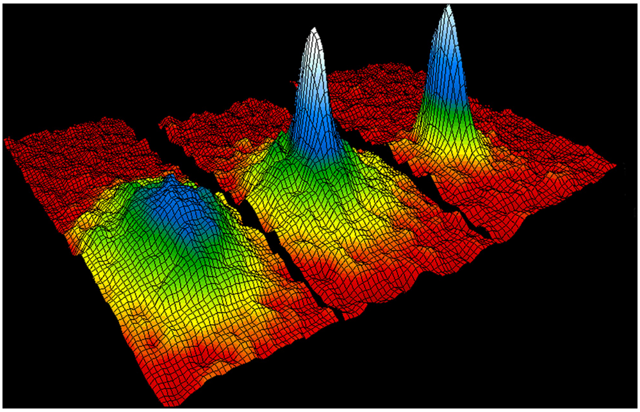

Fig. 1.18 – Transition to condensation: false-color images representing the velocity distribution of atoms at different temperatures: from left to right $T > T_c$, $T < T_c$ and $T \ll T_c$ (JILA, USA, Credit: Mike Matthews).

Finally, when approaching the absolute zero of temperature, we observe only a single distribution, very sharp, corresponding to the condensate. Since the atoms in the condensate all behave the same way, with the same velocity, the width of the velocity distribution depends on the interactions between atoms. Note that although we consider condensates, their density remains very low ($10^{19} - 10^{20}$ m^{-3}) compared to the density of a solid ($10^{28} - 10^{29}$ m^{-3}); they are always diluted gases.

The first condensates were obtained with alkaline atoms (rubidium, sodium), which have a single valence electron on their outer electron shell. Today, about fifteen chemical elements have been condensed: alkalis (lithium, sodium, potassium, rubidium, cesium), hydrogen, metastable helium, chromium, alkaline earth metals (calcium, strontium, barium) and rare earth elements, such as erbium, dysprosium and ytterbium. Note that we can also condense molecules, as we will see in chapter 7.

Bose–Einstein condensates (BECs) are very sophisticated physical systems because their realization requires the simultaneous implementation of many technological feats (ultrastable lasers, ultra-high vacuum below 10^{-10} mbar, very high quality optical elements, vibration-isolated devices, complex computer-driven time sequences, etc.). In the early 1990s, only a few of the more experienced laboratories could obtain a condensate. Nowadays, a large number of atomic physic laboratories have a BEC, and this in almost all the developed countries of the world. These quantum systems hold such riches that they have become basic tools for solving a considerable number of crucial problems in physics, as the following chapters will show.

1.3.3 Atom Boxes Made of Light

The trapping and manipulation of ultra-cold clouds or condensates are based on the principles we have seen previously. In particular, optical traps are easy to set up with various geometries. By interfering two beams coming from the same laser source, we create a standing wave with nodes and bellies, *i.e.* a periodic intensity profile in space and therefore a set of regularly spaced optical traps called an optical lattice. The distance between the traps is on the order of the laser wavelength, typically on the order of a few hundred nanometers. When we place a cloud of cold atoms in such an optical lattice, we can divide it into smaller clouds, each trapped at the bottom of lattice site (see figure 1.19a). It is also possible to combine two or three pairs of laser beams, the beams of each pair interfering with each other but not with the beams of the other pairs. Two-dimensional or three-dimensional optical lattices are thus created: the first case corresponds to an optical "egg box", the second to a stack of egg boxes, in which the atoms are trapped. These networks are widely used in optical clocks (see chapter 2) and quantum simulations (see chapter 4); they exhibit certain analogies with the crystalline structure of solids.

It is also possible to "draw" the traps by taking advantage of the reaction time of the atoms. The idea is to move the focal point of the laser beam creating the optical trap very quickly with respect of the characteristic motion time of the atoms. We can move the laser beam continuously so as to make a ring (see figure 1.19b). It is also possible to operate discontinuously, in the manner of dotted lines: for each of the successive positions of the focusing point, the laser is switched on for a very short

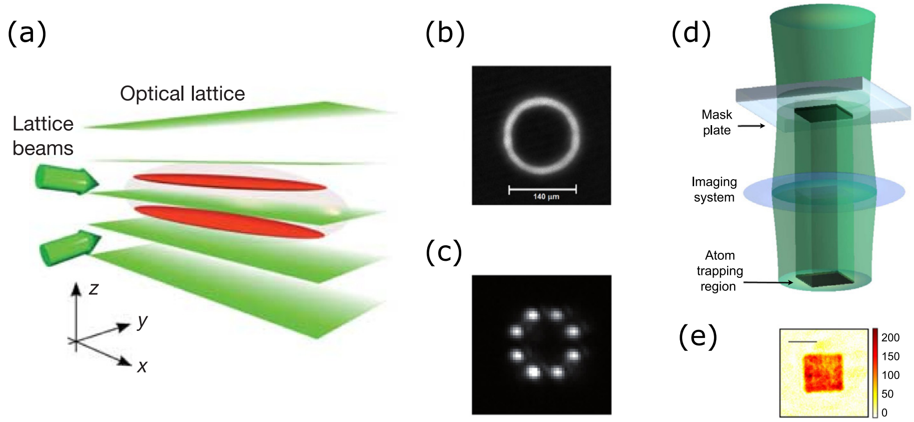

Fig. 1.19 – Examples of geometries of optical traps for ultra-cold atoms: (a) Schematic diagram of a one-dimensional optical lattice allowing to divide a cloud of ultra-cold atoms into two plane clouds (in red). Figure taken from Z. Hadzibabic *et al.*, *Nature* **441**, 1118–1121 (2006). (b) Atoms trapped in an annular trap. Figure taken from T. A. Bell *et al.*, *New J. Phys.* 18, 035003 (2006). (c) Atoms trapped in a ring lattice. The diameter of the ring is 6.9 μm. Figure taken from B. Zimmermann *et al.*, *New J. Phys.* **13**, 043007 (2011). (d) Schematic diagram of the production of a trap with a flat bottom, using an intensity mask which is imaged in the zone where the atoms are trapped. (e) Density of a uniform cloud trapped in a "square box" of side 30 μm. Figures (d) and (e) are taken from L. Chomaz *et al.*, *Nature Communications* **6**, 6162 (2015).

time. We can thus make a trap containing several wells in the manner of an egg box but arranged for example on a circle (see figure 1.19c).

In all these cases, the traps are based on an intensity profile which varies spatially and which has a parabola shape around the focal point. The consequence is that the clouds of trapped atoms have a non-uniform density. This can lead to difficulties in interpreting the experimental results and comparing them with developed theoretical models. It has been recently demonstrated that one can create optical traps with flat bottom, in which the clouds have a uniform density (see figure 1.19d and e): these traps are obtained by combining several laser beams and using intensity masks imaged in the atom trapping zone. These masks can be produced, for example, by means of a metallic deposit on a glass slide (see figure 1.19d) or using a spatial light modulator, which allows computer-control of the light intensity profile of a laser beam.

1.3.4 Atoms can Attract or Repel

Despite the low density of the cold atom gases, interactions between atoms, resulting from collisions between atoms, are at the heart of the properties of these ultra-cold gases. While collision modeling is usually a very complicated problem, working with ultra-cold gases greatly simplifies the problem. At low temperatures, we can only consider the lowest energy collisions and we are able to describe the interactions between atoms by so-called contact interactions, which only depend on a single parameter a, called the scattering length. In the case where a is positive, interatomic interactions are repulsive. In this case, the collisions between atoms can be seen as collisions between billiard balls. In the case where a is negative, interatomic interactions are attractive; we can no longer use the image of colliding billiard balls (this would amount to consider billiard balls of negative radius). If $a = 0$, we are in the case of gases without interaction. The sign of a plays an important role in the stability of condensates. If a is positive, condensates are stable; in this case, the repulsive interactions also lead to an increase in the size of the cloud compared to the case without interaction. If a is negative, condensates are stable only if they contain only a small number of atoms or if the trap is very large.

Experimentally, it is possible to modify the scattering length a and therefore to control interatomic interactions, *via* a phenomenon called Feshbach resonance (see also chapter 4). The scattering length a is tuned by applying a well-chosen homogeneous magnetic field on an optically trapped cold atom cloud. To obtain this magnetic field, two coils of the same axis traversed by identical currents in the same direction are used. The ideal configuration is the Helmholtz configuration where the distance between the two coils is equal to the radius of the coils. By applying the homogeneous magnetic field, it is then possible to modify the nature of the interactions: from attractive to repulsive and *vice versa*. For example, the rubidium-85 atom naturally has a negative scattering length a, which prevents the production of stable condensates containing a large number of atoms. By making the scattering length positive, this becomes possible. It is also possible to vary the scattering length from positive to negative very quickly in order to study the collapse of the cloud (see figure 1.20).

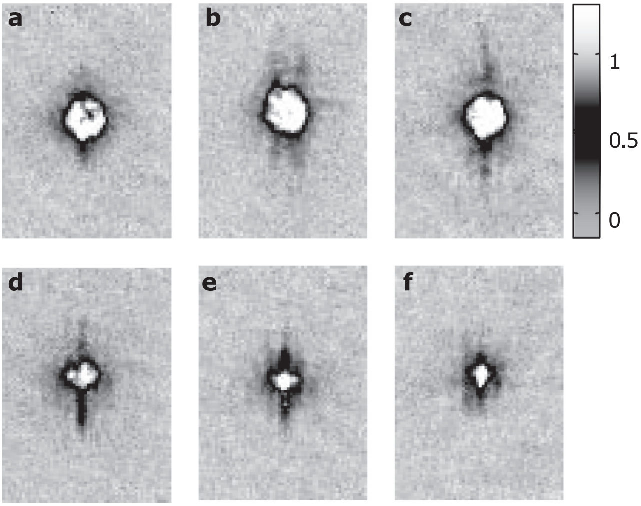

Fig. 1.20 – Collapse dynamics of a rubidium-85 condensate (images are taken for different times) following a sudden change from a positive scattering length a (repulsive interactions) to a negative scattering length (attractive interactions). The images (from a to f) are obtained for evolution times of 2, 3, 4, 6, 8 and 10 ms respectively. Each image is 0.150 by 0.255 mm in size. Figure taken from E. A. Donley *et al.*, *Nature* **412**, 295–299 (2001).

We will come back in more detail in chapter 4 on Feshbach resonances, the control of interatomic interactions being a very useful tool in the field of quantum simulation.

1.4 And the Whole Jungle of Particles on a Microscopic Scale

1.4.1 What is Matter Made of? Bosons and Fermions

There are two types of particles: bosons and fermions. These two types of particles are characterized by their intrinsic angular momentum or spin, which is a purely quantum property without equivalent in classical physics. Bosons have full spin and fermions have half spin. In particular, particles – protons, neutrons, and electrons – which constitute the atoms are fermions of spin 1/2. Depending on the number of their neutrons, atoms can thus be bosons or fermions. At high temperatures, bosons and fermions behave in the same way: we can consider them as point objects independent of each other, like marbles. At low temperatures, however, they behave differently; we say that they do not follow the same statistics (see figure 1.21): the Pauli exclusion principle states that two fermions cannot simultaneously occupy the same quantum state. Bosons, on the other hand, are not subjected to this principle and can accumulate in the same quantum state to form a Bose–Einstein condensate (see above).

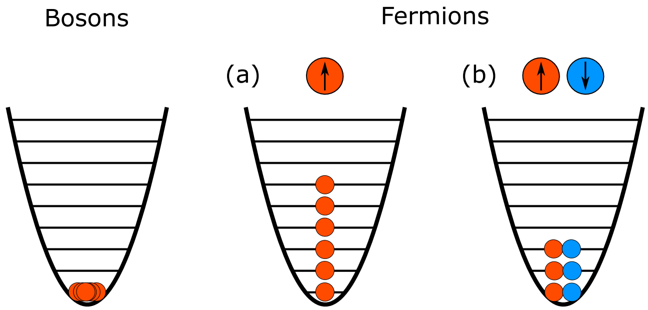

Fig. 1.21 – At zero temperature ($T = 0$ K), bosons and fermions do not behave in the same way: (a) bosons accumulate in the lowest energy state of the trap. (b) In the case of identical fermions (in the same internal state), the fermions populate the states of lower energies at the rate of one fermion per energy state of the trap, due to the Pauli principle. (c) In the case of non-identical fermions (in different internal states), the fermions populate the states of lower energies, at the rate of two fermions per energy state of the trap: one of each type.

1.4.2 Fermions can also Get Ultra-Cold

The first degenerate fermionic gas was obtained in 1999 in the group of D. Jin (JILA, USA), four years after the obtention of the first condensates (degenerate bosonic gas). The difficulty is that collisions between identical fermions (of the same internal state) are suppressed at low energy due to the Pauli exclusion principle. It is thus not possible to directly cool a cloud of identical fermions by the method of evaporative cooling. It is necessary to use what is called sympathetic cooling: we can for example make a mixture of bosonic and fermionic isotopes of the same species in the same trap (see figure 1.22). The bosonic cloud is cooled by evaporative cooling and thanks to boson-fermion collisions, the fermionic cloud sees its temperature decreasing. It is also possible to use a mixture of non-identical fermions, *i.e.* of different internal states: indeed the collisions between non-identical fermions are not suppressed, even at low energy. At very low temperatures, all the fermions populate the states of lower energies and form a Fermi sea. This state is close to that of electrons, which are also fermions, in solids. Thus, ultra-cold fermions are of great interest for the simulation of condensed matter properties (see chapter 4). In the case of a fermion gas with strong attractive interactions, the fermions can pair and thus form bosonic molecules, which can condense (see chapter 7).

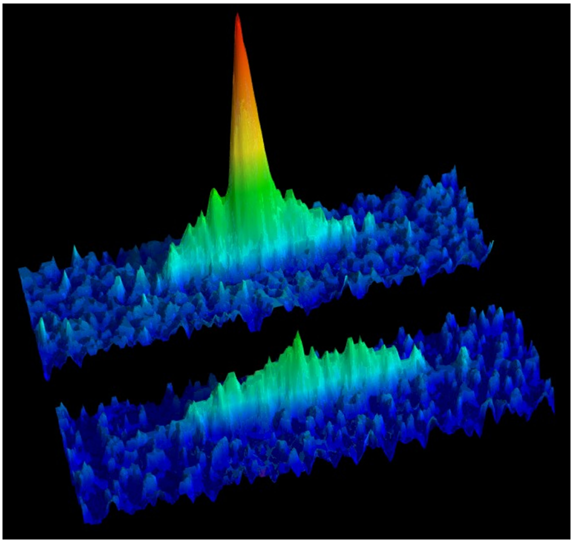

Fig. 1.22 – Bosonic and fermionic degenerate gases: false color images showing the velocity distribution of a bosonic cloud (Bose–Einstein condensate of lithium-7, top) and a fermionic cloud (Fermi sea of lithium-6, bottom) (Fermi gas team, Ecole normale supérieure, Paris).

1.5 Conclusion

This chapter has presented the mechanisms of laser cooling of atoms to reach temperatures on the order of a few microkelvin in milliseconds *via* momentum exchange with laser light. These atoms can then be trapped in a wide variety of traps created using magnetic or light fields. The Bose–Einstein condensate is then obtained when the atomic ensemble reaches extremely low temperatures of the order of the nanokelvin. These ensembles of ultra-cold atoms are created in a perfectly controlled and isolated environment. This gives experimentalists an extremely large degree of control over these systems. The geometry of the trap, the temperature of the atomic cloud, the statistics of atoms (fermions or bosons), their collisional properties or the presence of impurities are all available parameters. In the following chapters, we will see how these ensembles of cold atoms are used to carry out high precision measurements, defining the state of the art for some of them, or to simulate complex systems, with in particular a large number of interacting particles, emanating from other fields of physics, such as solid-state physics or astrophysics.

Chapter 2

Cold Atom Instruments and Metrology

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At very low temperatures, the motion of atoms obeys the laws of quantum physics: as we have seen in the first chapter, atoms are no longer point-like particles, but small wave packets that can propagate freely or be confined in traps in which their motion is quantized. The wave nature of this motion allows the realization of very precise sensors: atomic clocks that measure time, or atomic interferometers that measure gravity, acceleration or rotation.

These devices are currently complex instruments, designed, developed and constantly improved in research laboratories around the world. In France, this research is notably carried out at the Observatoire de Paris. The very high precision measurements offered by these devices enable an ever increasing number of applications, as the technological barriers fall. We can thus not only deepen our knowledge of the fundamental laws of physics that govern our Universe, but also better understand the internal structure of the Earth.

Finally, sensors based on cold atoms are beginning to emerge from the isolated basements of laboratories to be used commercially or to be embarked in satellites.

2.1 What is Metrology?

2.1.1 Concepts of Statistical and Systematic Uncertainty

Metrology is the science of measurement. Any measurement of a physical quantity, such as length, mass or time, is subject to error due to the imperfections of the measuring device. We categorize these errors according to whether they are

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systematic or random. In the former case, the error remains the same from one measurement to the next — it is due to a wrong calibration of the measuring device — and thus introduces a bias in the measurement. It is generally possible to understand the origin of this bias, and thus to correct for it, but this understanding is inherently limited. The uncertainty on the correction to be applied to the measurement is called the "systematic uncertainty", it affects the "*accuracy*". In the latter case, the error has the form of a random fluctuation, which we call "noise", and whose amplitude is called the "statistical uncertainty" and limits the "*stability*" of the device. Fortunately, this fluctuation can be averaged and thus disappear by averaging a large number of measurements. However, depending on the required accuracy, accumulating enough measurements may take some time, which may be prohibitive.

2.1.2 Atoms as References

Metrologists have long used artifacts as references for their measurements. The prototype for the meter was a bar of platinum-iridium whose length was chosen as the 40th of the circumference of the Earth. Pendulum clocks, then quartz clocks, tuned to the movement of the Earth gave the time. And until 2018, the International Prototype of the Kilogram kept at the Bureau International des Poids et Mesures in Sevres weighed, by definition, exactly 1 kg. However, these artifacts have a fundamental problem: they are imperfect because they are man-made. They are not exactly reproducible, are sensitive to the environment (temperature, pressure), and are altered by aging: these perturbations make these references inaccurate.

For this reason, metrology has turned step by step to quantum physics to find better standards. First by redefining the meter from the wavelength of radiations emitted by atoms, then the second *via* a transition of the cesium atom. The last iteration of these evolutions of the Système International of units (SI), adopted in 2018, defines the seven base units that make it up, including the meter, the second, the kilogram and the ampere, by fixing the numerical value of fundamental constants, in particular the numerical value of Planck's constant h, the characteristic scale of the quantum world. Thus, units are no longer attached to contingent artifacts, but to our deep knowledge of the laws of microscopic physics.

In this microscopic world, atoms are ideal systems for making precision measurements. From a fundamental point of view, all atoms of the same species are rigorously identical and unalterable. Their properties, uniquely determined by the laws of physics and the associated fundamental constants, are independent of the person handling them. They are therefore perfectly adapted to play the role of absolute standards, independent of any human construction, as the physicist James Clerk Maxwell had already anticipated in 1870. From a practical point of view, atoms, thanks to laser cooling and manipulation techniques, can be efficiently isolated from their environment, thus drastically reducing measurement biases, which allows for accurate measurements. Finally, the laws of quantum physics that describe them offer an interesting property: the energy of an atom can be quantized, *i.e.* it can only take certain particular values, which can be used as a reference.

2.1.3 Metrology with Quantum Systems

While quantum physics is ideal for building accurate measurement devices, it imposes a fundamental limit on the stability of the measurement: the result of a measurement with a quantum system necessarily includes some randomness. For example, measuring the energy of an atom that is in a superposition between two quantum states provides a result that is randomly the energy of one or the other of the two states. However, as we will see later, such a measurement is a basic principle common to all quantum sensors. This randomness introduces a noise in the measurement: it limits the stability of the device.

To overcome this limitation, it is possible to simultaneously probe a large number of atoms, and thus to average the noise, in the limit where the interactions between the atoms do not disturb the measurement outcome. Another method, more exploratory, consists in generating and manipulating collective quantum states of the atoms used in the measurement device. These techniques, which are very difficult to implement, are common with the research topics pursued to realize quantum computers and quantum simulators.

2.2 Atomic Clocks

Introduced in the 1960s, atomic clocks are the best devices able to measure time, so that the unit of time of the International System, the second, is defined since 1967 from a microwave resonance of the cesium atom. Since the adoption of this definition, the performances of atomic clocks have improved continuously, reaching a control of their frequency at the level of 10^{-16} (*i.e.* we are confident that the first 16 digits of the clock frequency are not subjected to perturbations) for cesium clocks. Even better: for the last ten years, clocks using other types of atoms, the optical clocks, have surpassed the cesium clocks and are now 100 times better.

2.2.1 Principle of an Atomic Clock

Atomic clocks are all based on the interaction between a gas of atoms and an electromagnetic wave. This interaction makes it possible to imprint the frequency of the oscillation of the electrons around the nucleus of the atoms on the oscillation of the electric field of the electromagnetic wave. The latter can then be measured to compare clocks with each other. This principle is detailed in figure 2.1. The performance of the clock must then be evaluated. First, the frequency stability is measured by comparing the residual frequency fluctuations of two independent clocks. Once the sources of technical instabilities are under control, the stability of the clock remains limited by the quantum projection noise (figure 2.2). Finally, the accuracy of the clock is evaluated by estimating the effect of external perturbations on the energy levels of the atoms. These perturbations are most often of electromagnetic nature, for example as a result of the influence of an external magnetic field, of static electricity in the vicinity of the atoms, of molecular interactions between atoms that are too close to each other, or finally *via* the presence of residual light arriving on the atoms.

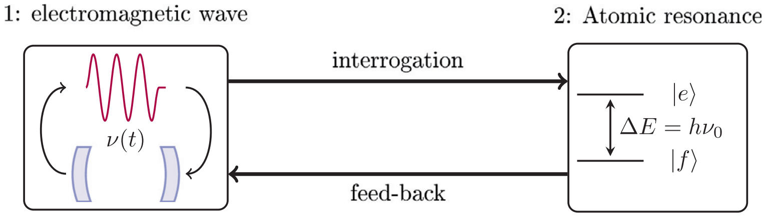

Fig. 2.1 – An atomic clock consists of two components: first, a local oscillator composed of an electromagnetic wave whose frequency $\nu(t)$ is pre-stabilized on a macroscopic resonator such as a cryogenic sapphire crystal or a resonant optical cavity; second, a set of atoms having an adequate transition between two quantum states of the electrons orbiting an atom. The atom interacts with the electromagnetic wave, and thus can only change quantum state if the frequency $\nu(t)$ of the electromagnetic wave is tuned with the natural frequency ν_0 of the atomic transition, defined from the energy difference ΔE between the two states *via* Planck's relation $\Delta E = h\nu_0$. Then, a system able to detect the state in which the atom is allows, *via* a servo method, to keep the electromagnetic wave at resonance: $\nu(t) = \nu_0$.

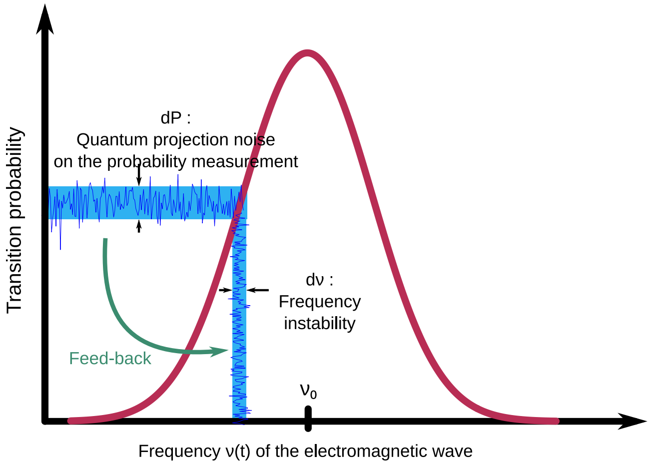

Fig. 2.2 – Illustration of the quantum projection noise that limits the frequency stability of atomic clocks. We represent on this figure probability p that the atom changes state as a function of the detuning between the frequency of the electromagnetic wave $\nu(t)$ and the natural frequency of the atom ν_0. This curve has the shape of a resonance: the probability is maximal when the detuning is zero. The quantum nature of electronic states necessarily introduces a random outcome to the measurement of this probability, with a deviation dP that is smaller when a large number of atoms are probed simultaneously. This randomness, called the "quantum projection noise", is converted into noise $d\nu$ on the frequency of the electromagnetic wave, *via* the feed-back system locking the frequency of the electromagnetic wave to the atomic transition.

In particular, the ultra-high vacuum chamber in which the atoms are contained emits infra-red radiation due to its temperature — this is the black body radiation. This radiation modifies the properties of the atoms, and thus the frequency of the atomic clock. This frequency must therefore be corrected according to the temperature of the environment, within the limits of our knowledge of the latter.

2.2.2 Why Use Cold Atoms?

Beyond the electromagnetic effects, the main systematic disturbance in the operation of an atomic clock is due to the movement of atoms, *via* the Doppler effect. Because of the movement of the atoms, the frequency of the electromagnetic wave appears smaller or larger depending on whether they are moving away from or towards the source, just like the tone of a siren emitted by a moving vehicle changes according to the speed of the vehicle. While the first atomic clocks used vapors or jets of atoms at room temperature, which are still in use in most commercial compact clocks as well as for the clocks on board certain satellites, the best laboratory atomic clocks now use cold atoms to achieve the best performance. This technology has allowed a significant improvement of atomic clocks since its first use in the 1990s.

2.2.3 Cold Cesium Atom Clocks

In cold cesium atom clocks, a set of laser cooled atoms, produced in an optical molasses or in a magneto-optical trap, with a temperature of the order of a microkelvin is launched vertically by transferring them momentum with laser beams (figure 2.3). The atoms rise and fall along a ballistic trajectory, in the same way as any other object in motion in the earth's gravitational field. Because of the resemblance between the trajectory of the cold atoms and the trajectories of vertically launched water drops, these clocks are called "atomic fountain clocks". During their trajectory, the atoms interact with an electromagnetic wave in the microwave domain, lasting longer the higher the trajectory. The longer the interaction time, the better the resolution with which the frequency of the atomic resonance can be measured, according to the Fourier principle. Most atomic fountains have a height of the order of a meter, which leads to an interrogation time on the order of a second. Finally, a differential detection system is used to determine the fraction of atoms transferred to the excited state of the clock transition. This information is fed into a servo system that tunes the frequency of the electromagnetic wave to the atomic resonance. After several decades of development, the control of systematic effects, *i.e.* the accuracy of cesium clocks, has reached the level of 10^{-16}: after one year of operation, these clocks only deviate by a few billionth of a second. Their stability is limited by the quantum projection noise (figure 2.2) which introduces relative frequency fluctuations of the order of a few 10^{-14} from one second to another. These fluctuations average out over time, reaching a statistical resolution of 10^{-16} after a few days of operation. In the world, some of these clocks are in operation almost continuously, and are used in particular to calibrate the international time scale TAI (Temps Atomique International) on which is based the

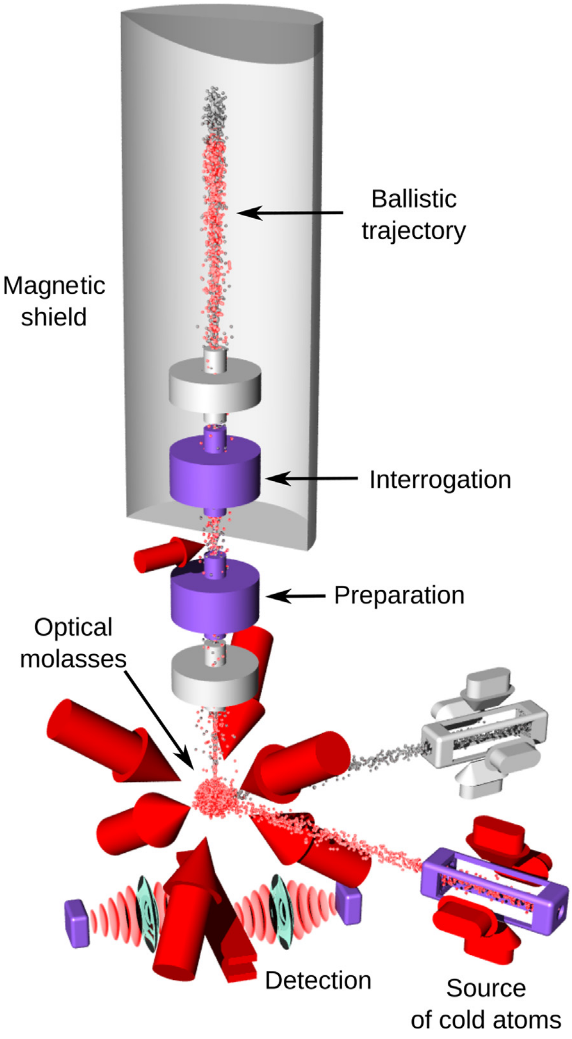

FIG. 2.3 – Schematic of an atomic fountain. A set of cold atoms is prepared by laser cooling (in an optical molasses or a magneto-optical trap). The atoms are launched on a ballistic trajectory during which they interact with the electromagnetic wave in a microwave cavity. At the end of their trajectory, a set of lasers measures the quantity of atoms transferred to the excited electronic state as a result of the interaction. The atomic fountain depicted here, developed at LNE-SYRTE at Paris Observatory, operates with cesium atoms, as primary frequency standard, but also simultaneously with rubidium atoms (shaded part on the diagram). This double fountain allows to measure very precisely the frequency ratio between the two atomic species, for instance in order to perform fundamental physics tests (see paragraph 2.4).

Coordinated Universal Time (UTC), in use in most countries of the world. An offset of a few seconds between these two time scales allows to keep UTC synchronized with the rotation of the Earth, to compensate for the irregularities of the latter. However, it seems difficult to improve significantly the accuracy and the stability of atomic fountains, as their limitations are fundamental.

2.2.4 Trapping Atoms to Improve Accuracy

One of the limitations of caesium clocks remains the effect of the motion of the atoms. Despite all the care taken to cancel the Doppler effect in atomic fountains, the residual velocity of the atoms causes systematic effects, limiting the accuracy at the 10^{-16} level, and it would be very difficult to improve on this. Fundamentally, the uncertainty arises from the fact that probing the clock transition does not only change the energy state of the electrons of the atoms, but also slightly changes the motion of the atoms. To improve the clocks, one must then use trapped cold atoms instead of free cold atoms. If the trapping is achieved with a sufficiently large force and in a sufficiently small region of space — this is the so-called "Lamb-Dicke" regime — the motion of the atoms in the trap can no longer be described by the laws of classical physics, as would be the case with a classical object attached to a spring, but by the laws of quantum physics. Thus, the mechanical energy associated with the motion of the atoms can only have a few very specific values, or quantum states, which are well separated from each other: the motion of the atoms themselves is quantized in terms of motional states, like the motion of the electrons around the nucleus. If we ensure that the process of interrogating the atoms by the clock's electromagnetic wave does not cause the atom to change from one motional state to another, we guarantee that the motion of the atom has no influence on the frequency of the clock.

2.2.5 Optical Clocks and the Future Definition of the Second

Optical clocks are a new generation of clocks that use trapped atoms. In addition, the frequency of the clock resonance is 10 000 times greater than the frequency of caesium clocks, so that the electromagnetic wave interacting with the atoms is merely a laser beam in the visible range. These two features combined make these clocks already 100 times better than caesium clocks, both in terms of accuracy, on the order of 10^{-18}, and stability, on the order of 10^{-16} after one second of operation, so that an optical clock can measure in one second an effect that would take a whole day to measure with a caesium clock. Furthermore, the fundamental limits of these clocks are not yet known, and their improvement is still in progress. The trapping techniques used in these clocks depend on the nature of the atomic species used. In order to trap neutral atoms, such as strontium, ytterbium, or mercury, we use optical lattices (figure 2.4), whereas we trap ions in radio frequency traps (Paul traps, see chapter 6). Clocks with neutral atoms offer the advantage of being able to probe tens of thousands of trapped atoms at the same time, whereas it is still very difficult to trap several ions in close vicinity to each other without disturbing them

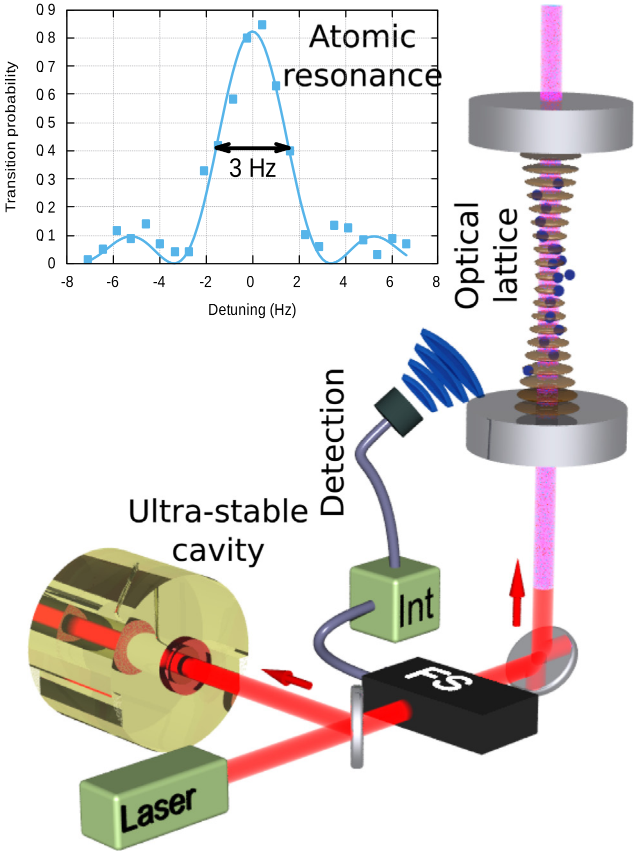

FIG. 2.4 – Scheme of an optical lattice clock with strontium atoms. In these clocks, the atoms are trapped in an optical lattice made of a thousand of light wells formed by a standing laser beam in an optical resonator, less than one micrometer apart. The atoms are interrogated by a clock laser pre-stabilised on an ultra-stable cavity, and their excitation is detected by fluorescence.

in a prohibitive way. Therefore, neutral atom clocks are equivalent to ten thousand ion clocks operating in parallel: the imperfections that are different for each of the atoms are thus reduced by an averaging effect, such as the quantum projection noise that limits the ultimate stability of the clock.

Progress in the field of optical clocks suggests that, in the near future, the second of the International System of units (SI) will have to be redefined based on these clocks. The Comité International des Poids et Mesures has issued a list of criteria that these clocks must meet before a possible redefinition, in terms of not only performance, reproducibility, and contribution to TAI, but also means of comparison between these clocks on a continental or even global scale.

2.2.6 Links between Clocks and Time Scales

Caesium clocks can be compared remotely using GPS signals which contain time information. This is how the TAI and UTC time scales are constructed. However, these satellite methods are not sufficient to take full advantage of the accuracy and stability of optical clocks. It takes several days of measurements before the frequency noise from the GPS clocks and the propagation of the signals in the Earth's atmosphere can be averaged out to the 10^{-16} level. In order to compare distant optical clocks, it is therefore necessary to establish ground-based comparison methods. Fort this purpose, several European metrology institutes are now connected by optical fibres. The challenge of transmitting a clock signal by fibre is to cope with the attenuation of the signals, and the perturbations introduced by the fibres, arising from thermal and mechanical perturbations. In order to overcome these problems, metrological fibre network methods are able to cancel phase fluctuations *via* a round trip in the fibre, coupled with the use of bidirectional optical amplifiers. These links are now used to compare optical clocks with resolutions a thousand times better than satellite methods, and with an integration time of only a few hours.

2.3 Atom Interferometers

The quantum superposition principle can also be exploited to build atomic interferometers which are no longer sensitive to the transition frequency between two levels of the atom, but rather to the inertial forces which apply to it. Here the quantum states that will interest us are those of the external motion of the atoms, determined by the position and the velocity of the atoms, as opposed to the internal motion, linked to the energy of the internal electronic states of the atom. In this paragraph, we describe the operating principle of these interferometers, the different types of very high sensitivity inertial sensors that they allow to achieve, as well as some of their applications.

2.3.1 Principle of an Atom Interferometer, Similarities and Differences with a Cesium Atomic Clock

Atomic interferometers exploit the wave nature of matter and the possibility for matter waves to interfere. Atoms do not only behave like particles, but also like wave-packets, which we can separate and recombine, as we can do with photons in optical interferometry. To manipulate atomic wave-packets, physical tools similar to beamsplitters and mirrors that are used in optics are needed, but adapted to atoms. It is in particular possible to use material diffraction gratings, formed by a series of slits of widths on the order of a hundred nanometers.

But the most effective tool for manipulating atomic wave-packets remains the interaction with laser beams. Indeed, as we saw in the first chapter in figure 1.2, when an atom, of mass m, and initially in an electronic state f and in a state of momentum $p = mv$, absorbs a photon which allows it to change electronic level, it also absorbs its momentum. When the excited state e has a sufficiently long lifetime, a light pulse at wavelength λ of duration and intensity correctly adjusted, will place the atom in a superposition state of the two quantum states: the first with energy level f and momentum p and the second with energy level e and momentum $p + p_a$, where $p_a = \hbar k$ is the momentum of the photon and $k = 2\pi/\lambda$ is the wavenumber of the laser. These two states, which have velocities that differ by a quantity $\hbar k/m$, called the recoil velocity, are like those of two partial wave-packets (of a same atom!) which will therefore separate spatially during the free evolution which will follow the interaction with the light pulse. For an alkaline atom, such as rubidium or cesium, this recoil velocity is of the order of a few mm/s, so that at the end of a free flight of the order of a second, the two wave packets are separated by a macroscopic quantity, of the order of several millimeters. In practice, we most often use not one-photon transitions, but two-photon transitions, in which atoms change their electronic state by exchanging two photons with a light field made up of two lasers which propagate in opposite directions. This arrangement of beams, presented in figure 2.5, creates an optical lattice, like those of the previous chapter in which we can trap the atoms, but which we are going to light on here for a very short time, of only a few microseconds, and on which the matter waves will diffract, like photons on material gratings, see figure 2.5.

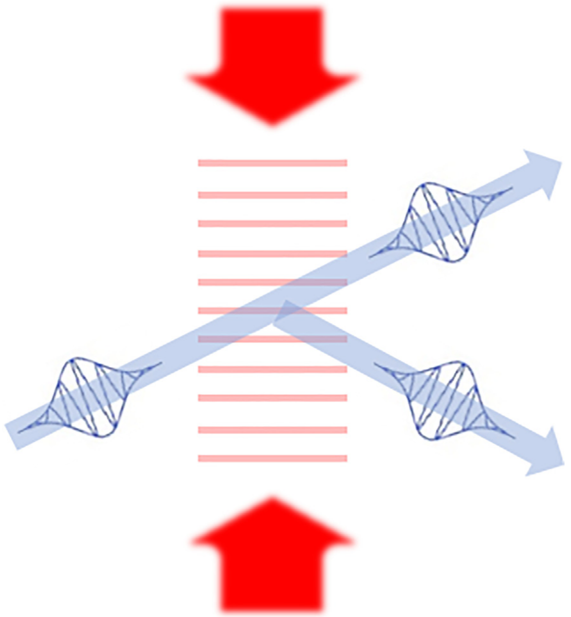

Fig. 2.5 – Under the action of a laser pulse, produced here using two laser beams propagating in opposite directions, the atom, here represented as an incident wave packet, is placed in a quantum superposition of two partial wave packets, the first transmitted and the second reflected (or diffracted). These two wave packets have different velocities and will therefore separate spatially during the free flight phase which follows the light pulse.

But to realize an interferometer, it is still necessary to recombine these partial wave-packets. For this, a laser pulse sequence is used. Using three pulses, separated by free evolution times T as long as possible, we can respectively separate, redirect and recombine the wave packets, as shown in figure 2.6. The first and third pulses are analogous to beamsplitters, while the middle pulse acts as mirrors, which redirect the wave packets to each other after they have separated. The state of the atoms at the output of the interferometer is again a superposition of the two partial wave-packets partial wave-packets, which will therefore again, after the third pulse, separate, constituting the two output ports of the interferometer. In this two-wave interferometer, the probability of detecting atoms in each of the two output ports depends on a phase, the phase of the interferometer, which is given by the phase difference accumulated by the matter waves along the two paths (we speak of the two arms of an interferometer).

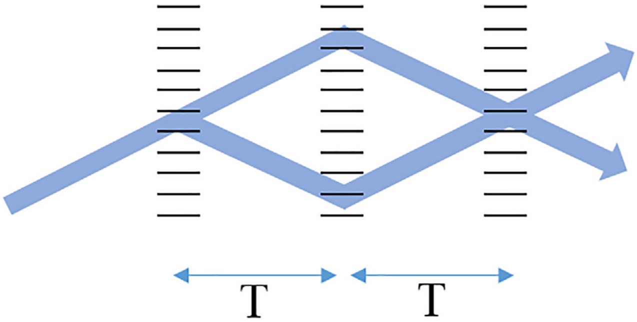

Fig. 2.6 – A sequence of three laser pulses, separated by free flight times of duration T, makes it possible to produce an atomic interferometer. The first and last pulses play a role analogous to beamsplitting plates in optics, while the middle pulse acts as a mirror for the matter waves.

This type of atomic interferometer is sensitive to physical effects which may affect the two arms in different ways, and in particular to interactions with electromagnetic or inertial fields. The sensitivity of the measurement will generally depend on the physical separation between the two arms, and therefore on the delay $2T$ between the input and the output of the interferometer. Here again, the use of cold atoms is decisive, since it makes it possible to increase this delay, which is designated as the duration of the interferometer. A very common and seminal instrument architecture is therefore very similar to that of microwave clocks. We start by preparing a sample of cold atoms, which we release in free fall, and which we can in certain experiments launch upwards as in atomic fountains to maximize the duration of the interferometer. Then, instead of a series of microwave interactions, a sequence of laser pulses is carried out, which creates the atomic interferometer, then the populations in the two output ports are detected using a detection similar to that of clocks.

2.3.2 Inertial Sensors Based on Atom Interferometry

As atoms are sensitive to inertial forces, the trajectories of the two arms of the interferometer, in which the atoms are in fact in free fall, are affected in the reference frame of the instrument (and in a different way) by the accelerations and the rotations undergone by the experimental device. In particular, the phase of the interferometer not only depends on the acceleration along the direction of the laser beams used to manipulate the wave packets, but also on the rotation perpendicular to the plane which encompasses the two arms of the interferometer. This is what enables inertial sensors such as accelerometers and gyrometers to be produced using these interferometers.

One of the advantages of these atomic inertial sensors is that their scale factor, which is the ratio between the measured physical quantity (for example a voltage or a current, here a phase) and the inertial quantity that interests us (for example an acceleration or a rotation rate) is perfectly stable. It is here linked to the parameters of the interferometer lasers, to the duration of the interferometer or even to the velocity of the atoms. For example, the phase related to the acceleration a is given by $\phi = kaT^2$. Now, we can determine (and control) the wavevector k, which is related to the frequency of the laser, as well as the duration T with excellent precision, as good as that of the best atomic clocks if necessary. This guarantees the accuracy and stability of the acceleration measurement, at much better levels than for conventional accelerometers, whose scale factor, which drifts over time, must be regularly calibrated.

Moreover, these atomic sensors are extremely sensitive. For a duration $2T$ of the interferometer of only 200 ms (which corresponds to a fountain height of only 5 cm), we obtain for rubidium atoms a phase of more than one million radians for an acceleration equal to g, the acceleration of gravity. For a measurement noise of this phase of the order of a thousandth of a radian (which typically corresponds to the limit set by detection noise in this type of sensor), we obtain a sensitivity on the measurement of g of 6.10^{-10} in relative value. We can therefore use these methods of atomic interferometry to produce gravimeters, that is to say instruments which measure the acceleration of gravity and its variations, spatial and temporal. To do this, we throw upwards or drop the atoms, and align the laser beams of the interferometer along the vertical direction (see figure 2.7).

In practice, the measurement noise is largely dominated by ground vibrations, which must be rejected with the greatest possible efficiency. The sensitivities of the best atomic gravimeters are in the end on the order of 5.10^{-9} g at 1 s measurement time. By averaging consecutive measurements, one can resolve variations in the acceleration of gravity as small as 5.10^{-11} g (roughly the acceleration corresponding to the gravitational pull of a mass of 10 kg placed 1 m below or above the sensor). We can easily see that with such sensitivities, we can, by producing maps of g, detect density anomalies in the subsoil, linked to the presence of cavities, fluid reservoirs (gas, oil) or mineral deposits. By following the temporal evolution of g, we can still study mass transport phenomena, such as the emptying of hydrological reservoirs or the rise of magma in a volcano.

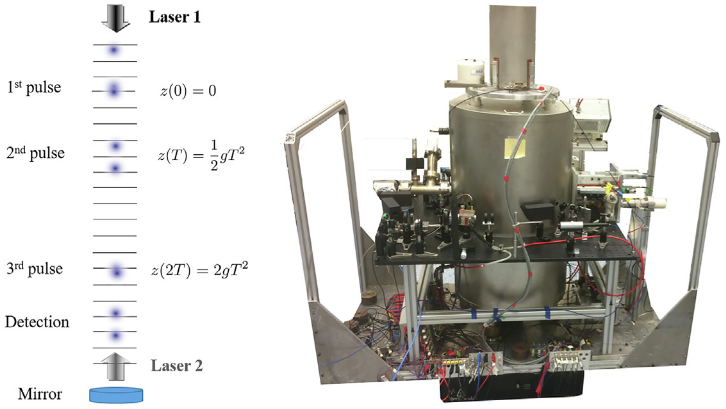

Fig. 2.7 – Left: Trajectories of atomic wave packets in an atomic gravimeter. The interferometer lasers, which are aligned along the vertical direction, separate, redirect and recombine the wave packets, which are then detected by fluorescence. Right: Photograph of the free-fall chamber of the SYRTE gravimeter. The vacuum chamber rests on an aluminum plate, placed on a vibration isolation platform. It is surrounded by a cylindrical magnetic shielding which isolates it from the disturbances of external magnetic fields. A seismometer which measures the residual vibration noise is above the shielding. A laser system for generating ultra-cold atoms is placed around the shield. (Courtesy of Sébastien Merlet).

It is also possible, using other arrangements of the laser beams and other trajectories of the atoms, to measure accelerations along the horizontal directions, or rotation rates along different directions. Other pulse sequences can also be used to optimize the sensitivity of the sensor to a particular inertial quantity of interest. For example, a 4-pulse configuration, carried out on atoms launched in a fountain over a height of more than a meter, made it possible to reach stabilities for the measurement of rotation rates at levels which rival the state of the art of the best fiber gyrometers (which are however much more compact). But, new methods of beam-splitters, which we will mention later, or the confinement of atoms in guides, could make it possible to increase the sensitivity and reduce the size of the sensors, thus opening the way to new uses in the most natural field of application for this type of instrument that constitutes inertial navigation.

The sensitivity of interferometers to inertial forces can also be exploited to make measurements of differential acceleration, that is to say the difference in acceleration between two clouds of atoms interrogated by the same laser beams. This is the geometry used to measure the gravity gradient (an atomic gradiometer is produced with two interferometers spaced apart along the vertical, typically a few tens of cm). This instrument configuration has the considerable advantage of effectively rejecting vibration noise, because it disturbs the measurements of the two interferometers in the same way and disappears when the difference of the two acceleration measurements is made. They can therefore be used to perform gravity measurements in disturbed environments, in the field or on board carriers (planes, ships) to perform gravity field mapping covering large areas. It is even envisaged to embed this type of sensor in satellites in low orbit to produce a complete map of the Earth's gravity field, with a spatial resolution and a precision better than that obtained with missions using electrostatic accelerometers. These gravity measurements from space make it possible to better understand the movements of mass on the Earth, linked to the dynamics of the internal and external layers of the Earth (circulation of magma, volcanism, ocean circulation, drainage of hydrological basins). These gradiometers have also been used to determine Newton's gravitational constant by atomic interferometry, by measuring the disturbance of the gravity gradient caused by the presence of large, well-known test masses. We also use accelerometers in differential mode to carry out tests of Einstein's equivalence principle, the consequence of which is that all bodies subjected to the same gravitational field (to the exclusion of any other external force, and therefore in void) fall simultaneously when simultaneously released, regardless of their internal compositions. The principle of measurement therefore amounts to comparing the accelerations felt by two atoms of different species, for example rubidium and potassium.

Another remarkable application of atomic interferometry is the extremely precise measurement of the recoil velocity of an atom. Here, the momentum of a large number of photons, on the order of a thousand, is transfered to the atoms and their change in velocity is measured extremely precisely using an atomic interferometer. This measurement of the recoil velocity allows *in fine* one of the most precise determinations of the fine structure constant, which is the dimensionless constant which characterizes the strength of electromagnetic interactions.

2.3.3 Maturity of the Sensors and Industrial Transfer

Almost thirty years after the first demonstration experiments, and after more than twenty years of in-depth studies of their performance limits, atomic sensors based on atomic interferometry today enjoy good technological maturity and have, for some, demonstrated better performance than conventional state-of-the-art. This is particularly the case with atomic gravimeters, for which there is no lack of concrete applications. Various institutes have embarked on the development of transportable cold atom gravimeters, more compact, to facilitate their deployment in the field. The first measurement campaigns outside the laboratory have already taken place, in particular for measurement sessions on a fixed site, in geodetic observatories or for comparison campaigns of absolute gravimeters, or for measurement campaigns on board carriers (boat and plane). Key technologies have also been the subject of industrial transfers. Atomic gravimeters are now marketed by the French company Muquans (see figure 2.8), which has relied for the development of its instruments on research carried out at the Paris Observatory and the Institut d'Optique. The first units have already found buyers for applications mainly in geosciences: gravity measurements in geodetic observatories, field measurements for hydrology, vulcanology.

FIG. 2.8 – Photograph of the atomic gravimeter marketed by the company Muquans. On the left, the laser bench and the control electronics. On the right, the drop chamber in which the cold atoms are in free fall.

2.3.4 Novel Architectures

However, these successes do not mean that research in the field is finished, quite the contrary. While it is true that the limits of instruments based on laser-cooled atoms and on two-photon transitions are now well understood, new avenues still largely remain to be explored to overcome these limits.

In particular, the accuracy of the measurements is limited by the phase and intensity inhomogeneities of the interferometer laser beams, to which atoms are sensitive because they move in these beams during of their free fall due to their residual ballistic expansion. The use of better quality beams, but especially of much colder atoms, whose temperatures are in the range of tens of picokelvin rather than microkelvin, and for which the ballistic expansion is much smaller, will make it possible to limit the biases linked to these inhomogeneities.

The sensitivity of the measurement is for its part ultimately limited by the separation of the arms of the interferometer and by the detection noise, two parameters on which it is still possible to act. To increase the separation, we can certainly increase the interaction time, by building very large devices (several 10 m tall fountains are under development), but we can especially improve the efficiency of the beamsplitters, by imparting to atoms a much greater momentum than those of one or two photons. And it is possible, using pulses based on high order diffraction processes, and on sequences of such pulses, as well as on the acceleration of atoms in moving optical lattices. Today, using these tools, we can already transfer, as illustrated in the figure 2.9, the momentum of several hundred photons, and the demonstration of gains remarkable in sensitivity will not be long in coming. Finally, to reduce the detection noise, it is envisaged to use as sources clouds of atoms which

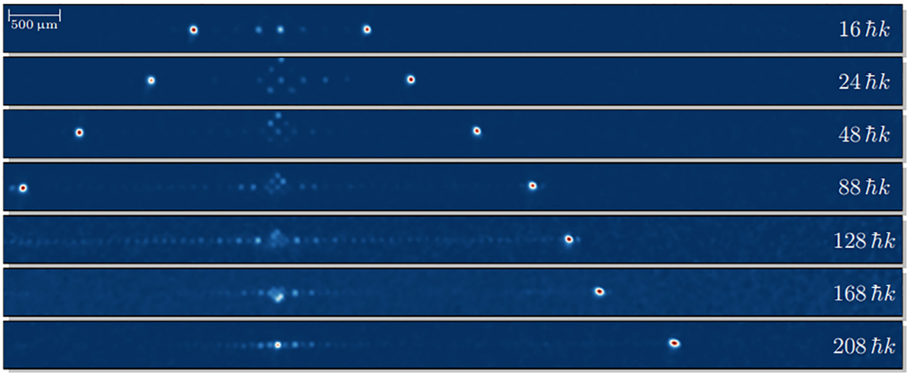

Fig. 2.9 – Spatial separation of wave packets after different large momentum transfer beamsplitters. The greater the momentum transfer, the greater the separation of the wave packets. The atoms are detected here by absorption imaging after a period of free flight after their interaction with the beamsplitters: they are then illuminated with a laser beam, the intensity of which is absorbed where the atoms are located. (Courtesy of Sven Abend, Leibniz University of Hanover).

present particular quantum correlations (we speak of compressed spin states or spin squeezing). In the presence of such correlations between the atoms, the quantum fluctuations of the measurement are weaker than when one averages the result of the measurement on a set of N independent atoms: the sensitivity then improves as $1/N$, instead of $1/\sqrt{N}$. This method is presented in more details in chapter 3.

The use of these new tools (ultra-cold atoms, more efficient beamsplitters, correlated states) should make it possible to increase the sensitivity of the instruments by several orders of magnitude or to reduce their size, opening the way to the most ambitious applications. We can mention, in addition to autonomous navigation and measurement of the gravity field from orbiting satellites, the detection of dark matter or the detection of gravitational waves in frequency bands not covered by optical detectors, present or future, using differential acceleration measurements in atomic interferometer networks, on baselines several kilometers in length.

2.4 Probing the Fundamental Laws of Physics with Cold Atom Sensors

We have seen that measurement devices based on cold atoms achieve accuracies that no other measurement device can reach. Therefore, they allow numerous applications in both fundamental and applied physics, such as satellite positioning systems, like GPS, which were made possible at the time of their development by the development of onboard atomic clocks.

2.4.1 Gravimetry and Chrono-Geodesy

Gravimetry, which is the study of the effects of gravity generated by the Earth, is an application of atomic interferometers, but also of atomic clocks. To understand how a clock, which measures time, is sensitive to gravitation, one must appeal to Einstein's general theory of relativity. This theory states that time does not elapse in the same way at all locations, but rather depends on the gravitational potential. The flow of time is thus distorted by the proximity of large masses like the Earth. This effect follows directly from the equivalence principle which states that the effects of acceleration cannot be distinguished from the effects of gravitation: as the effect of the former is to shift frequencies *via* the Doppler effect, the latter must also shift frequencies (figure 2.10). This effect is commonly called the "gravitational redshift", referring to the fact that frequencies are reduced by gravitation. For example, a clock that is lowered vertically by one metre on the Earth's surface will have its frequency reduced by 10^{-16} in relative units. This effect is therefore easily observed with atomic clocks, and the construction of a global time scale such as International Atomic Time must take it into account because the different clocks that contribute to these time scales may be located at very different altitudes. However, while altitude, in the gravitational sense of the term, is well determined locally by geophysicists *via* altimetry or satellite positioning methods, it is difficult to establish consistently at the continental scale to better than a few centimetres. This is where optical clocks can come in: comparing distant optical cold atom clocks with an accuracy of 10^{-18} will allow the gravitational potential difference, *i.e.* the altitude difference, to be measured

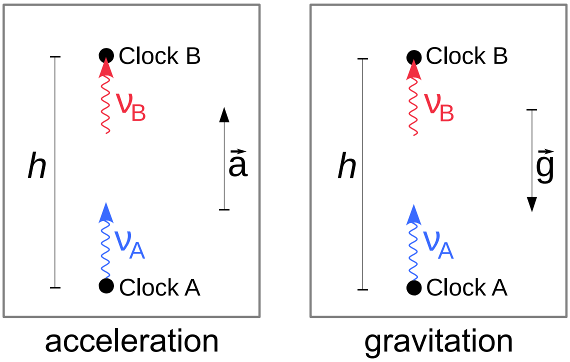

Fig. 2.10 – Gravitational redshift. In the situation depicted on the left, two accelerated clocks separated by height h are compared by sending an electromagnetic signal from clock A to clock B. Due to acceleration, the speed of the clocks on reception and transmission are different. Thus, because of the Doppler effect, the frequency of the electromagnetic wave is smaller at the receiving end, by an amount ah/c^2. It is said to be red-shifted. Einstein's equivalence principle states that acceleration and gravitation cannot be distinguished (situation shown on the right). This is why clocks located at different altitudes in a gravitational field are detuned by a quantity $gh/c^2 = \Delta W/c^2$ where ΔW is the gravitational potential difference between the two clocks (Credit: P. Delva, SYRTE).

with an accuracy of 1 cm. Such comparisons would provide geophysicists with unprecedented information about the Earth's gravitational potential, *i.e.* about the Earth's internal structure. Such measurements with clocks would be complementary to those made with gravimeters: while a cold atom gravimeter is sensitive to the gravitational field, which decreases as the inverse of the square of the distance between the structure generating the field and the measuring device, a clock is sensitive to the gravitational potential, which decreases simply as the inverse of the distance. Thus, a clock would give information about deeper structures in the Earth's mantle.

2.4.2 General Relativity and Gravitational Waves

Instead of precisely measuring small variations of the gravitational red shift at the Earth's surface, it is also possible to measure it on a larger scale, for example by comparing a stationary clock on Earth with a clock on a satellite. The frequency shift then becomes so large that its agreement with the prediction of general relativity can be checked with unprecedented accuracy. This is one of the objectives of the Pharao/ACES space mission, during which a cold caesium atom clock will soon be embarked on the International Space Station. For 18 months, the frequency of this clock will be compared with the frequency of the best terrestrial clocks, providing an unprecedented tests of general relativity (figure 2.11).

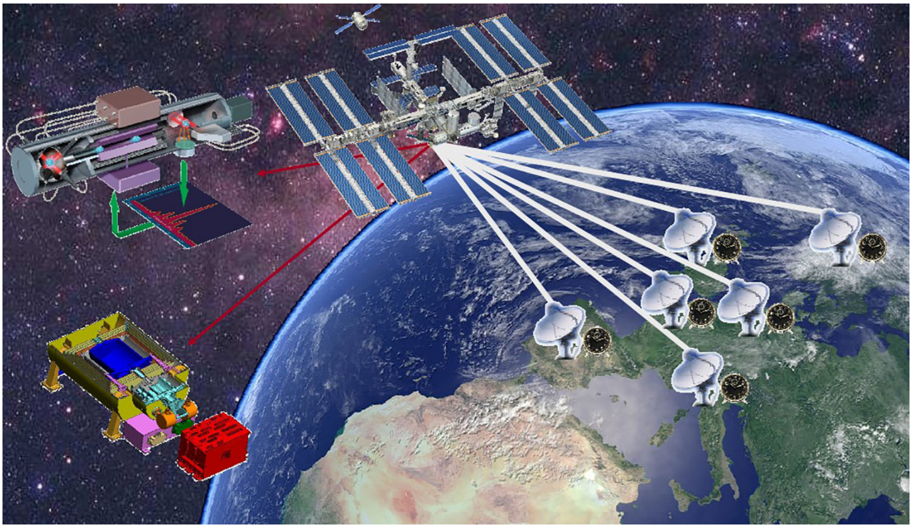

Fig. 2.11 – The Pharao cold atom space clock experiment (top left) will be part of the European Space Agency's Atomic Clock Ensemble in Space (ACES) mission aboard the International Space Station (ISS) (schematic: L. Cacciapuoti, ESA). In zero gravity, atoms can move freely for an extented duration as compared to atoms on Earth, thus increasing the accuracy of the caesium clocks. By taking advantage of the high altitude of the ISS, it will be possible to test the gravitational shift of general relativity in an unprecedented way, by comparing the Pharao clock with optical clocks on the ground *via* a microwave link.

Another consequence of general relativity is the existence of gravitational waves generated by astronomical cataclysms, which propagate in the intergalactic medium and eventually arrive on Earth, where they almost imperceptibly disturb the measurement of distances. These waves have been detected for some years by the LIGO and VIRGO detectors, in which laser beams measure variations in distance between mirrors with a resolution at the 22nd decimal place. The passage of the gravitational wave, through the deformation of space–time that it induces, causes this distance to slightly oscillate in accordance with black hole merger models. However, these detectors cannot detect lower frequency waves because their signal is overflown by the residual vibrations of the mirrors, which are of seismic origin. To solve this problem, it is possible to insert atomic interferometers into the arms of a gravitational wave detector. The distance reference would then be cold atoms in free fall in vacuum, which, unlike mirrors, are not subject to ground vibrations. The aim of the MIGA project is to produce a first prototype of such a detector as a proof of principle. More prospectively, it has also been proposed to detect gravitational waves with a constellation of satellites in space carrying very high precision optical clocks, but such an application is still futuristic.

Other experiments yield tests of the special theory of relativity. This theory states that in the Universe, no direction is privileged. For example, the speed of light is a constant, regardless of the direction from which it comes. This hypothesis can be verified by comparing optical clocks on a continental scale *via* optical fibre links: because of the rotation of the Earth, clocks located at different locations evolve at different speeds with respect to the rest of the Universe (figure 2.12). Thus, the observation of a difference in frequency between clocks varying during the course of a day would be a proof of the violation of the hypothesis of invariance of the speed of light. On the contrary, the absence of such an observation allows to put more and more restrictive bounds on a possible violation of this invariance. Such tests have already been carried out in Europe, and the continuous improvements of optical clocks will allow to further improve these tests.

2.4.3 Standard Model and Dark Matter

While the standard model of particles describes with an astonishing accuracy all the physical phenomena observed on Earth, in particular in particle detectors, it is challenged by astronomical observations which highlight the existence in galaxies of matter, of unknown nature for the moment, which interacts with ordinary matter by the gravitational interaction. However, the particles constituting this unknown matter are not "visible" because they do not interact, or very little, with ordinary matter *via* the electromagnetic interaction, nor even *via* nuclear interactions. These particles are thus called "dark matter".

Because cold atom sensors are among the most sensitive measurement devices, they could offer an opportunity to detect a possible interaction between ordinary matter and dark matter, and, as a consequence, to characterize the latter. Indeed, through this hypothetical interaction, the passage of dark matter through the Earth would modify the usual properties of ordinary matter, and thus the results of certain measurements such as the values of frequency ratios between atomic clocks using

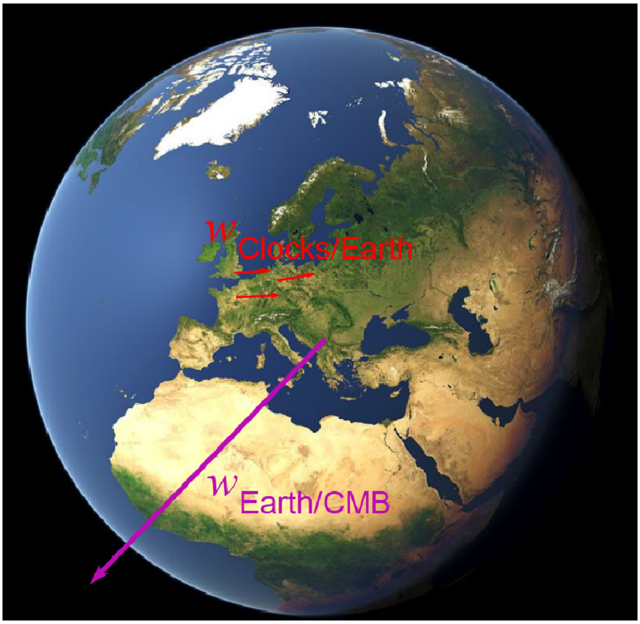

FIG. 2.12 – Comparing optical clocks swept along in space by the rotation of the Earth, which itself travels at several hundreds of km/s in the galaxy, makes it possible to verify the principle of isotropy of the speed of light: the frequencies of the clocks must not depend on the movement of these clocks with respect to a hypothetical privileged reference frame such as the reference frame of the Cosmological Microwave Background (CMB), a remnant from the Big–Bang. This figure shows the comparison of three optical clocks, located in France, Germany and the United Kingdom, which, *via* their different longitudes and latitudes, move with different speeds throughout space. To date, these comparisons provide one of the most extensive tests of this invariance principle.

different atomic species. Several simultaneous international comparison campaigns between optical atomic clocks have already allowed to put upper limits to this phenomenon, in the framework of some dark matter models. In the future, global networks of atomic interferometers will improve on these attempts to detect dark matter.

Chapter 3

Single Atoms and Single Photons: Quantum Information Exchange

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We know the matter thanks to light. The presence of a body is revealed to us by the light it diffuses towards our eyes, or by the light it hides when it casts a shadow. Atoms are no exception to this rule: since the beginnings of quantum mechanics, almost all information we have about their existence and properties comes to us through their interaction with light (see figure 3.1). Thanks to cold atoms, it has become possible to observe individual atoms one by one, to use them as carriers of quantum information, and to put them in entangled states without classical equivalent. What happens to individual atoms and photons in these situations?

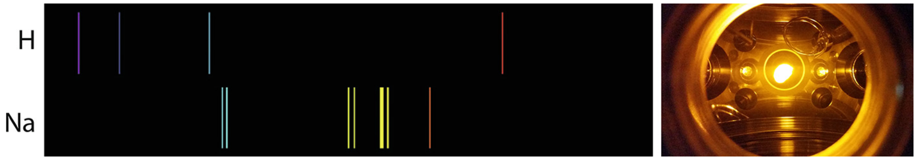

Fig. 3.1 – Left: emission spectra of hydrogen (top) and sodium (bottom). Each color corresponds to an atomic resonance. The rest of the visible spectrum is neither emitted nor absorbed by this atom. The spectrum is the fingerprint of the atom, each atomic species having a spectrum of its own. The observation of these spectra became possible at the end of the 19th century; it played a key role in the discovery of quantum mechanics. Right: fluorescence image of a cloud of sodium atoms cooled by laser in a vacuum chamber (see chapter 1). The cloud in the center of the image contains 600 million atoms at a temperature of 300 μK. The orange color of the cloud corresponds to the most intense emission line of sodium visible in the spectrum on the left (A. Schwettmann, University of Oklahoma).

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3.1 How to See a Single Atom

To see an object is to see how it transforms the light that illuminates it, by absorbing and diffusing it. These processes originate at the level of the atoms that constitute the object. In principle, nothing prevents us from seeing a single atom. Why, then, did not our teachers show us individual atoms in high school, under a microscope? The problem is twofold: on the one hand, the amount of light absorbed and emitted by a single atom is small, and on the other hand, atoms in a gas like air, at room temperature, move at high speeds, escaping from the field of view far too quickly for a detector to capture a large number of these photons. In 1953, when quantum mechanics was already firmly established, the great physicist Erwin Schrödinger could still state that "we never work with a single electron, atom or molecule. We sometimes pretend to do so in thought experiments, but this invariably leads to ridiculous consequences." In addition to showing that even the greatest scientists can be wrong, the quote testifies to the difficulty of isolating and observing a single quantum particle. Today, thanks to laser cooling and trapping, single atoms are part of the "toolbox" of quantum research. Observing them is the first step.

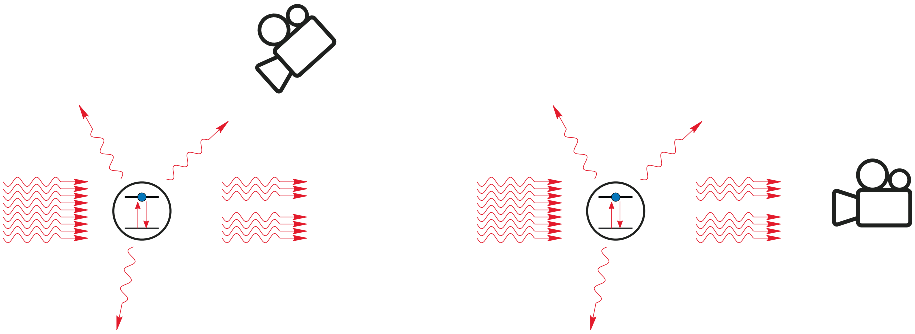

Fig. 3.2 – An atom illuminated by a resonant light beam (wavy arrows) absorbs photons, then re-emits them by spontaneous emission in random directions. To detect or even image the atom, we can collect the spontaneous photons (detection by fluorescence, on the left) or the attenuation of the beam (detection by absorption, on the right). Note that in both cases, the atom undergoes the recoil of the absorbed and emitted photons. We will see in the following a third method in which this recoil is absent.

When an atom is illuminated by a resonant light beam — that is, whose color corresponds to one of the atomic resonances — it absorbs a photon of the beam, then re-emits it by spontaneous emission. This emission, also called "fluorescence", occurs in a random direction, independent of the direction of the beam (see chapter 1). To detect the presence of the atom, we have two possibilities (see figure 3.2): either to place a detector in a transverse direction, to catch a part of the fluorescence photons, or to detect the attenuation of the incident beam, by placing the detector in this beam downstream of the atom. Both methods have their pros and cons, as we will see.

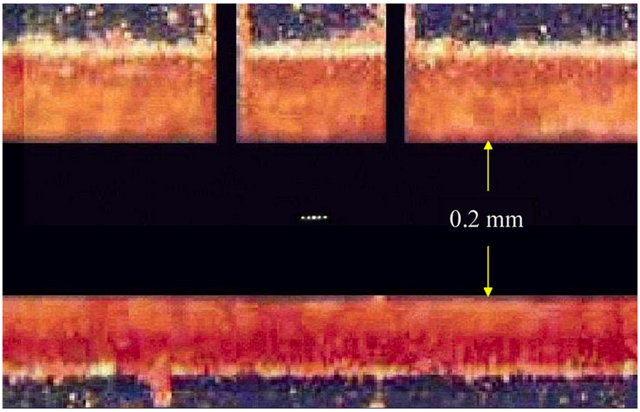

Fig. 3.3 – Photo of five beryllium ions suspended in vacuum between the electrodes of an ion trap. The ions are illuminated by a laser beam, of which they absorb a small part to re-emit it by spontaneous emission in all directions of space. On the picture, we do not see this beam because it is not directed towards the camera. On the other hand, a small part of the spontaneous emission goes towards this camera, which is sufficient to see the ions very clearly in the center of the image (D. Wineland, NIST Boulder).

Historically, it is in ion traps (see chapter 6) that this feat was first accomplished. Ions being charged particles, they can be trapped by the Coulomb force which is very strong. Thus, an ion remains trapped even after having undergone the recoil of a large number of absorbed and emitted photons. Figure 3.3 shows a picture of five beryllium ions suspended in vacuum between the electrodes of an ion trap. The ions are illuminated by a resonant laser beam, what we see is the fluorescence of each of the ions.

Neutral atom traps are much weaker. In order to see a single neutral atom, researchers had to find gentler, more photon-efficient methods that do not shake it up as much. A first idea is to detect absorption rather than spontaneous emission. Indeed, an image like the one in figure 3.2 only uses the photons incident on the camera's entrance lens — a small fraction of those emitted by the atom, the others having left in other directions without contributing to the image. When measuring absorption, on the other hand, each photon absorbed and emitted contributes to the useful signal: it is the "shadow" of the atom that constitutes the signal. The presence of the atom is detected by the attenuation it produces in the illuminating beam. But this attenuation is not complete: part of the photons cross the interaction zone without being absorbed, and constitute a background on the detector. If this background is too large, its fluctuations may hide the signal. Therefore, in order to work well, this method requires the most complete absorption possible. An atom absorbs photons that pass through its "cross section", an imaginary disk around the atom, whose radius is on the order of the resonant wavelength. If a photon passes at a distance smaller than this length, the atom will absorb it, otherwise, the photon is transmitted. To maximize the absorption, the beam must be focused until the size of the focal point is close to the cross section — an extreme focus, which requires a very sophisticated lens, custom-designed for this task. Figure 3.4 shows an experiment done in 2017 at the National University of Singapore (NUS) that uses this method. A single atom is laser cooled and trapped between two very good aspheric lenses. A tunable laser beam passes through the first lens, which focuses it on the atom. The second lens then sends it to a photodiode. The curve shows the photodiode signal when the laser frequency is swept across the atomic resonance. Far from resonance, the beam crosses the area without absorption, the signal of the photodiode is maximum. When the laser frequency reaches resonance, the atom absorbs up to 18% of the intensity, which is sufficient to detect its presence with a good signal-to-noise ratio. The difficulty of such an experiment comes from the atom's low probability of absorption: to obtain a result like the one in figure 3.4, one needs to focus the beam to the limit of what is possible, using the best microscope objectives available, while trapping the atom exactly at the focal point. And even then, as this experiment shows, the absorption is far from complete.

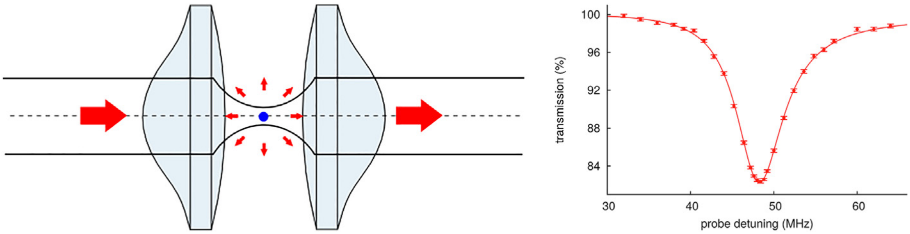

Fig. 3.4 – Detection of a single atom by absorption. Left: The atom is laser cooled and trapped between two converging lenses. A laser beam is focused onto the atom by the first lens, then collected by the second. When the laser is resonant with the atomic transition, part of the laser photons are absorbed by the atom and then scattered in all directions by spontaneous emission. The beam is thus weakened. A photodiode (not shown on the picture) detects the photons remaining in the beam. Right: Percentage of photons remaining in the beam as a function of laser frequency. The frequency is measured against a reference, the atomic resonance corresponds to 49 MHz on the abscissa. When the laser is tuned to this frequency, it is attenuated to 82% of its non-resonant intensity, the missing 18% correspond to the absorption of the single atom. This signal is easily detectable: the experimental noise is almost indistinguishable on the figure. This beautiful result is made possible by the combination of a good mastery of cold atom trapping and a very powerful optical system (C. Kurtsiefer, National University of Singapore).

3.2 The Benefit of Cavities

To counter this problem and obtain a complete absorption, we can use an optical cavity (figure 3.5). In such a cavity, a beam entering through one of the mirrors can travel a large number of times. Placing atoms inside a cavity dramatically increases their absorption probability due to these multiple passages. This effect has been exploited for a long time in spectroscopy, to detect gases in low concentration for example.

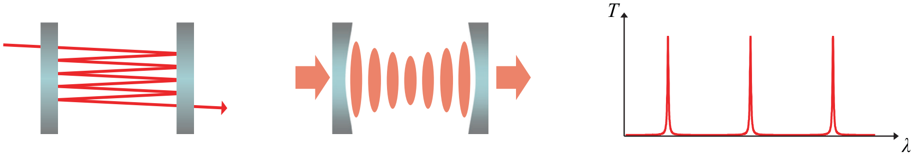

FIG. 3.5 – Principle of an optical cavity. Left: the light entering through the first mirror goes back and forth between the two mirrors facing each other. At each reflection, the mirrors let pass a small fraction of the beam. In the image, we have chosen a small angle to separate the different round trips. In reality, the incident beam is aligned with the axis of the cavity, so that all reflections are perfectly superposed. Center: when the length of the cavity is a multiple of the half-wavelength, a resonance phenomenon occurs. The different reflections are superposed in phase, forming a standing wave of large amplitude in the cavity. Out of resonance, on the other hand, they cancel each other on average. In that case, the field in the cavity remains weak, and the transmission as well, and the result is as if the second mirror was absent: the beam is almost completely reflected by the first mirror. Right: when we vary wavelength λ of the incident beam, we observe transmission T each time the resonance condition is met. At each successive resonance, the number of zeros of the cavity field changes by one.

With the cavities used in spectroscopy, however, the losses of the mirrors are too big and the optical field extends over too large a volume for the single-atom and single-photon effects to play an important role. The opposite regime — the most interesting one from the quantum point of view — is the one called "strong coupling". In this regime, each photon entering the cavity is absorbed by the atom, then re-emitted in the cavity mode, re-absorbed again, and so on. For this coherent energy exchange process to take place without being interrupted by the loss of the photon, cavities of a rare perfection are required. Indeed, the two sources of loss are the spontaneous emission of the atom (which makes the photon leave in another mode than the one of the cavity) and the imperfections of the mirrors (which can absorb the photon or diffuse it in any direction). We need to make the coherent coupling rate higher than the two loss rates.

To overcome spontaneous emission, the solution is to increase the coherent coupling rate by reducing the size of the optical mode in the cavity. This has two effects, both beneficial: first, the more the optical mode is focused onto the atom, the higher the coupling rate. Second, if the cavity mirrors cover a large part of the space around the atom, the cavity can also block some of the output modes that would normally be accessible to spontaneous photons, and thus reduce their rate. Observing quantum effects in the atom-photon coupling therefore requires miniaturized mirrors, bent to focus the mode, and placed at a sub-millimeter distance. To reduce the loss rate of these mirrors, their reflecting layer must be of extreme quality: no impurity must absorb the photon, no asperity in the surface must eject it from the cavity. In short, the cavity we are dreaming of is a real photon cage, similar to the “photon box” imagined by Einstein and Bohr in one of their thought experiments. Here, as is often the case, technological advance was the key to opening up a new field of research, the one known today as cavity quantum electrodynamics (CQED). The technological challenge was taken up by a handful of visionary researchers, who understood that it was necessary to “climb that hill to access the flowers in the valleys ahead”, as the American researcher Jeff Kimble put it. Two names are particularly associated with this field of research, that of Serge Haroche, winner of the 2007 Nobel Prize for his CQED work in the microwave field, and that of Jeff Kimble, who developed this field in the optical domain. Even if we cannot expose here all the richness of CQED research, one of its most emblematic manifestations is essential to understanding the role of cavities as single atom detectors. This is the Rabi doublet.

3.3 Strong Coupling Between a Photon and an Atom: The Rabi Doublet

What happens if we place an atom in a good cavity in the strong coupling regime? If the cavity is detuned from atomic resonance, the effect is simple: the presence of the atom shifts the resonant frequency of the cavity. This effect already exists in the weak coupling regime, even if it is smaller there. The sign of the shift — towards lower or higher frequencies — depends on the sign of the detuning — cavity frequency lower or higher than the atomic frequency. But what happens if the cavity is tuned exactly to the atomic resonance? For symmetry reasons, we expect neither an increase nor a decrease in the resonance frequency in this case. A very simple quantum model, introduced by Jaynes and Cummings at the beginning of the laser era, allows us to make a prediction: what should happen is a splitting of the resonance. The coupled atom-cavity system then has two resonances, called the “Rabi doublet”. These resonances are located on either side of the uncoupled resonance, and separated from it by the amount of the coherent coupling frequency (figure 3.6). In fact, an analogous resonance splitting also occurs in the classical world whenever two oscillating systems are coupled. What is fascinating here is the fact that a single atom and a single photon in the cavity are sufficient to produce it. When the incident laser beam is tuned to one of these resonance frequencies, light and matter form a “hybrid” state which is half photon, half atomic excitation. This happens thanks to the coherent energy exchange between these two strongly coupled entities. In the optical domain, the Rabi doublet was first observed in 1992 by Jeff Kimble and his team at the California Institute of Technology (CalTech). A more recent example is shown on figure 3.6.

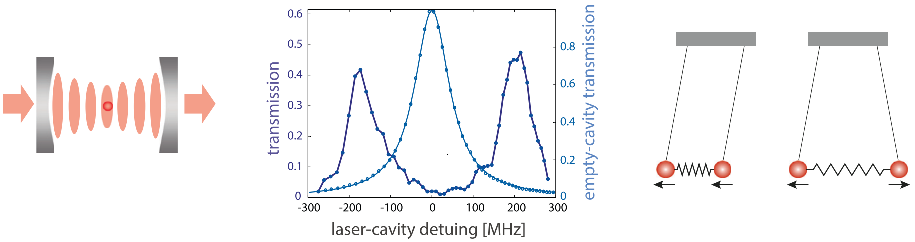

Fig. 3.6 – Rabi doublet. Left: we consider a single atom strongly coupled to a cavity mode. A probe beam of variable frequency is sent to the atom-cavity system and its transmission measured. The beam is very weak, such that at most one photon is in the cavity at a given time. Center: Transmitted intensity as a function of the laser frequency. Light curve: transmission of the empty cavity; bold curve: transmission in the presence of the atom. Instead of the single resonance of the empty cavity, we now observe two resonances: the Rabi doublet. The frequency difference between the two peaks of the doublet corresponds to twice the atom-photon coupling frequency (Roger Gehr, PhD thesis, Laboratoire Kastler Brossel/Université Pierre et Marie Curie, 2011). Right: a resonance splitting also occurs in classical systems where two oscillators are coupled. The image shows two pendula coupled by a spring. The oscillation of the coupled system occurs in two distinct "modes" shown in the figure. In the case of the Rabi doublet, a single photon is enough to cause this phenomenon.

3.4 The Atom Becomes a Qubit

The foundational experiments in cavity quantum electrodynamics were motivated by the desire to better understand the quantum world. In an unexpected way, they also helped to open a new field filled with promising applications: quantum information. In this field, an atom or other quantum object is considered as an elementary carrier of information. The specifically quantum phenomena — superpositions of states, non-classical correlation of several objects, measurement feedback — give rise to new, original and powerful methods of information processing (see box). The first step consists in using two atomic states to encode a binary information, $|0\rangle$ or $|1\rangle$. A natural way to do this is to use two stable internal states of the atom. These can be states of the spin, an atomic property that can be represented as a small arrow pointing up or down. Each of these two possible orientations corresponds to one of the two binary states, $|0\rangle$ and $|1\rangle$. The atom thus becomes a quantum memory, capable of storing a qubit of information. This qubit can take the value $|0\rangle$ or the value $|1\rangle$ like a classical bit, but it can also be in a quantum superposition of these two values, where each of the two states $|0\rangle$ and $|1\rangle$ has a probability amplitude. In atomic physics, researchers have been interested in these superpositions long before the advent of quantum information. Indeed, the same superpositions are prepared, for example, in atomic clocks, where they are used to measure an oscillation frequency specific to the atom (see chapter 2). Today, the concepts of quantum information make them shine in a new light. At the same time, atomic physics and the field of cold atoms in particular have an unparalleled toolbox to manipulate quantum information.

Qubits and quantum information

The information in our computers is stored and processed in binary form: the fundamental unit of information is a bit, which can take one of two possible values, $|0\rangle$ or $|1\rangle$. Any operation performed by a computer — whether it is photo editing or doing a mathematical calculation — can be described as a data transformation: the computer transforms an initial value ("input register") into a final value ("output register"). If we use a two-level quantum system to represent a bit — for example, a spin that can point up or down — then the principle of superposition applies, as it does for any quantum system. A quantum bit, or "qubit", can thus be in a superposition of both states, and in this sense it can be 0 and 1 at the same time. A quantum computer, which uses these qubits, is able in principle to perform the calculations corresponding to both values simultaneously! This is known as "quantum parallelism". However, the results of these parallel calculations are returned in the form of a superposition of states as well. To access them, it will be necessary to make a measurement, which will project the output register to only one of the possible results. Despite this, it is possible for some specific problems to exploit quantum parallelism and obtain an advantage over the best classical algorithms. This is the case in particular for integer factorization (Shor's algorithm).

Another peculiarity of the qubit is that reading it constitutes a measurement in the quantum sense, which thus causes a back action on the qubit and modifies its state. This fact can be exploited to protect data transmission against eavesdropping. Indeed, when a qubit is used in a communication system, it is impossible for an eavesdropper to know its value without leaving a trace. This is the basic idea of **quantum cryptography**.

3.5 Microcavities

Inspired by the new ideas of quantum information, researchers have developed a multitude of miniaturized optical cavities ("microcavities"), whose common goal is to concentrate the cavity's light field as much as possible in order to increase its coupling to atoms (figure 3.7). Each of these cavities has been designed to advance towards the perfect coupling between a photon — considered as a "flying qubit" — and a specific material qubit: atom, semiconductor quantum dot, diamond color center… On the other hand, once developed, each of these microcavities has found a multitude of applications, sometimes far beyond fundamental physics: new types of miniaturized lasers, frequency converters, filters for fiber telecommunications, etc. These are all examples of the hand-in-hand progress of fundamental research and new technologies.

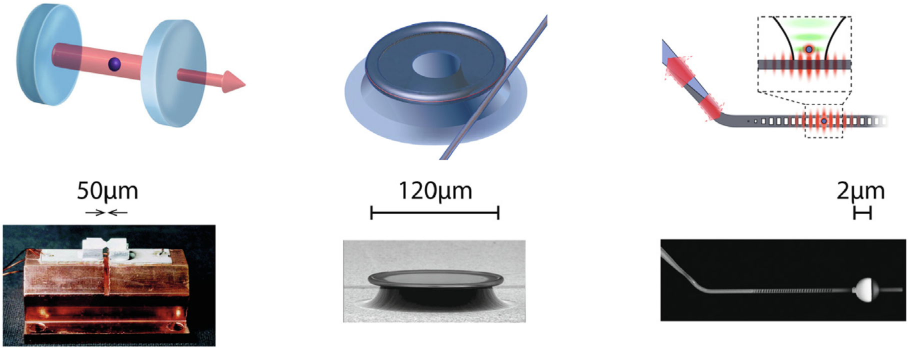

Fig. 3.7 – Different types of microcavities. For each type, the figure shows the principle (top) and a realization (bottom). The material used is the same in all three cases, fused silica (a glass of high optical quality). Left: Fabry–Perot cavity (see figure 3.5). In this type of cavity, the light field is localized in the free space between the two mirrors, which facilitates coupling to the atoms. In the photograph, the mirrors are the two pencil-shaped objects at the top of the image. The distance between their two surfaces, on the order of 50 μm, is too small to be visible in the photograph (J. Kimble, CalTech). Center: Toroidal resonator. Light propagates in a gallery mode along the circumference of the torus. Part of the optical field is localized inside the glass, the rest forms an evanescent wave at its surface. An optical fiber (shown in the schematic figure only) is used to excite the gallery mode (K. Vahala, CalTech). Right: One-dimensional photonic crystal cavity. The holes in the waveguide (horizontal part of the structure) are smaller than the wavelength. It is the presence of these holes that modifies the optical properties of the guide, transforming it into a cavity. Here as well, part of the electromagnetic field (red spots in the upper image) is located outside the glass (M. Lukin, Harvard). For this type of resonator, as for the toroidal resonator, coupling an atom to the field requires its trapping at a sub-micrometric distance from the surface. This trapping is possible with a very strong dipole trap (in green in the top image), but the proximity of the surface tends to reduce the lifetime of the atom and perturbs its energy levels.

One of these cavities with high application potential is known as FFP, for Fiber Fabry–Perot (figure 3.8). Since its inception in the author's team at Laboratoire Kastler Brossel in 2007, it has been adopted by several dozen laboratories around the world. This one is a cavity based on optical fibers. The principle is that of the optical cavity designed by Charles Fabry and Alfred Perot at the University of Marseille in 1897, which we have already seen in its macroscopic version (figure 3.5). The "Fabry–Perot" as researchers affectionately call it, is a very common optical instrument found not only in CQED experiments, but also in lasers, telecommunication networks, and even in some astrophysical telescopes. The novelty of the FFP lies in its miniaturized mirrors, which laser machined on the tips of optical fibers. The laser machining process allows realizing concave mirrors of micrometric size, while ensuring an excellent surface quality. The strong curvature of the mirrors allows the field to be concentrated in a minimal volume, while the extremely smooth surface minimizes losses. Additionally, the integration of the mirror onto an optical fiber results in an elegantly simple optical instrument. Indeed, by its very construction, the light propagating in the first fiber is automatically routed into cavity and then leaves it through the second fiber, without the tedious alignment that is normally required.

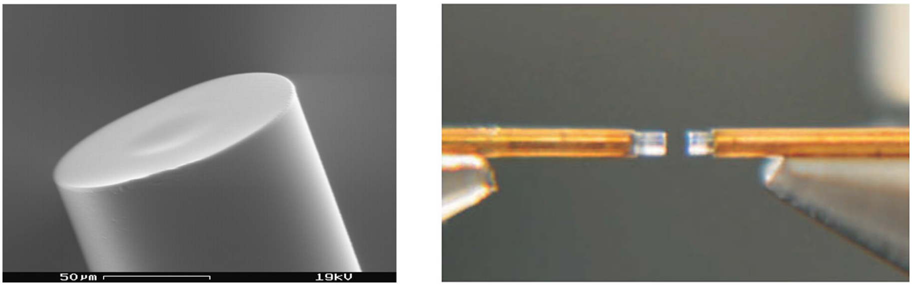

Fig. 3.8 – FFP (Fiber Fabry–Perot) microcavity. The principle is that of a normal Fabry–Perot cavity (see figure 3.5), but each mirror is fabricated on the tip of an optical fiber by laser machining. In this type of cavity, the light intensity is almost entirely localized in the free space between the two fiber mirrors. The mode volume is not quite as small as in a photonic crystal cavity, but the localization of the mode in free space allows obtaining better, perturbation-free coupling to an atom. Left: scanning electron microscope image of a fiber mirror. The image shows the tip of the optical fiber, which has a diameter of 125 μm. The concave depression in the center of the circular surface constitutes the mirror surface. Despite its inconspicuous appearance, this mirror has remarkable properties: its radius of curvature is about 100 μm, more than a hundred times smaller than what can be achieved with traditional superpolishing, while having comparable surface quality (Image: D. Hunger). Right: Image showing the principle of the cavity: two fiber mirrors facing each other form a miniature Fabry–Perot cavity. The light enters and exits through the fibers, a big advantage for its use in difficult conditions, such as in the vacuum chamber of a cold atom experiment (Image: B. Brandstätter).

3.6 Detecting the State of a Qubit

To be able to use atoms as qubits, first of all we need a way to measure the qubit state. This is a generalization of the single-atom detection problem, and cavity quantum electrodynamics can provide solutions. To actually make them work in real experiments, it was necessary to combine a clever application of CQED's physical mechanisms with the most advanced optical cavities. One of the best detectors is the one demonstrated at Laboratoire Kastler Brossel in Paris in 2010, using a cavity of the FFP type that we saw in the previous section. Figure 3.9 shows the principle of the experiment. The qubit is encoded in two sub-levels of the ground state of a rubidium atom, called hyperfine states. These two states are separated by an energy gap corresponding to a frequency of 6.8 GHz. The atom is trapped in the center of the cavity. The response of the cavity is measured in a very classical way: a probe beam is incident on the cavity, a first detector counts the transmitted photons, a

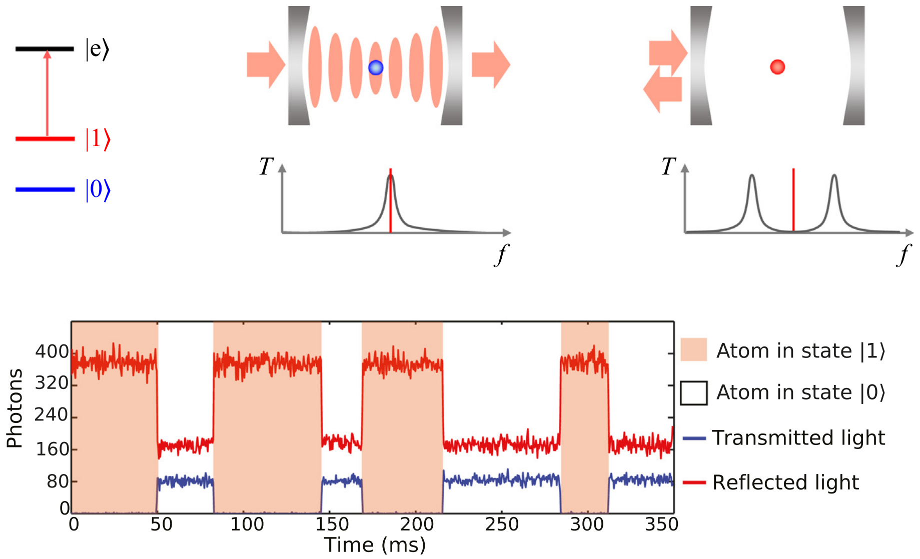

FIG. 3.9 – Detection of an atomic qubit without spontaneous emission. Top left: the atomic level diagram includes the two qubit states $|0\rangle$ and $|1\rangle$ as well as an excited state $|e\rangle$. The atomic qubit is placed in a fiber Fabry–Perot cavity, in the strong coupling regime, and illuminated by a probe laser. The cavity and the probe laser are tuned to the frequency of the $|1\rangle$ to $|e\rangle$ transition. Center: when the atom is in the $|0\rangle$ state, it is far from resonance with the laser and the cavity. Everything happens as if the atom was absent: the cavity transmits the probe beam. Right: when the atom is in the $|1\rangle$ state, we have the situation of the Rabi doublet (figure 3.6). As the laser is still at the frequency of the empty cavity, it is no longer resonant with the system, and is reflected by the first mirror. By detecting the transmission or reflection of the beam (or both), we can measure the state of the qubit. If it was in a superposition of the two states, the measurement projects it into one of them, randomly, according to the probability amplitudes of each state in the superposition. In contrast to the methods seen at the beginning of this chapter, this detection does not rely on spontaneous emission: if the atom is in $|0\rangle$, it is illuminated by the laser light, but does not absorb it because it is far from its resonance frequency. If it is in $|1\rangle$, it does not absorb either, because the light does not reach it. Bottom: photons recorded in transmission (blue curve) and in reflection (red curve) when the qubit alternates between the state $|1\rangle$ (periods marked by a pink background), and $|0\rangle$ (white background). Each of the signals allows to distinguish the two levels of the qubit with an excellent signal-to-noise ratio.

second one, those reflected by the cavity. The cavity is tuned to resonance with an optical transition that links the $|1\rangle$ state to an excited state. In fact, this is the same transition that is commonly used for laser cooling as described in chapter 1. The probe beam is also tuned to this frequency, and its intensity is low enough to have less than one photon in the cavity on average.

How does this arrangement allow us to detect the state of the qubit? Let us first consider the case where the qubit is in the $|0\rangle$ state. Thanks to the energy gap, this state is far from resonance and does not interact with the laser light. If the atom is in this state, everything happens as if it were not there: the probe beam is transmitted. If, on the other hand, the atom is in the $|1\rangle$ state, we are in the situation of the Rabi doublet (see figure 3.6). For the laser frequency, the resonance condition is no longer fulfilled. Therefore, the light is no longer transmitted, but reflected by the cavity's input mirror. Thus we see that the qubit atom acts as a switch, directing the flow of probe photons entirely to one or the other of the detectors, depending on its state. Figure 3.9 shows the signals from the two detectors while the qubit is made to randomly transit from one state to the other. The two states can be clearly distinguished with an excellent signal-to-noise ratio. To quantify the performance of this detector, we determine the detection error, *i.e.* the probability of detecting the state $|1\rangle$ while the atom is actually in the state $|0\rangle$, or on the contrary, of detecting it in $|0\rangle$ while it is in $|1\rangle$. In this experiment, 100 μs of detection is enough to determine the state of the qubit with an error below 0.08%, which established a new reference of high fidelity detection, never reached before for an atomic qubit.

3.7 Storing Quantum Information in Cold Atoms: Quantum Memories

The quantum memory is another key element of quantum technology. Its function is as simple to describe as it is difficult to realize: a quantum memory is a device which allows storing the value of a qubit and retrieving it at a later time. The task is much more difficult than the storage of a classical bit because for a single qubit (as for any quantum system), it is impossible, even in principle, to extract all information that it contains. A measurement of the qubit would give only one of the values $|0\rangle$ and $|1\rangle$, but not their probability amplitudes. Yet, these amplitudes constitute that invaluable information which sets the qubit apart from its classical cousin. What *is* possible, however, is to transfer the entire state of the qubit — that is, all information it contains — from one physical system to another. This is precisely the function of a quantum memory. The information arrives in the form of a "flying qubit" — a photon. The quantum memory transfers the information encoded in the flying qubit to a stationary, long-lived qubit. The latter can be an atom or another material system with two quantum states.

Quantum memories will be indispensable, in particular, in future long-distance quantum cryptography systems, which transmit secret information beyond a hundred kilometers or so. Quantum cryptography uses photons for transmission. Indeed, the photon being a quantum particle, it can also be used as a qubit carrier. The information can be coded in the presence or absence of the photon, or better, in a property of the photon such as its polarization. We can then transmit this photonic qubit by an optical fiber. However, just like the classical light used in current telecommunication, it undergoes attenuation during the transmission. In the classical case, it suffices to regenerate the signal every 100 km or so with the help of an amplifier. Ignored by most of us, these "repeaters" can be found along high-speed long-haul data lines, placed in booths near highways, for example where they ensure the transport of our web pages and streaming videos. For quantum information, the task is more delicate because of the fragility of quantum superpositions: even the theoretical feasibility a quantum repeater was not obvious *a priori*. Its theoretical demonstration is a relatively recent research result, dating from the early 2000s. It is these quantum repeaters that require quantum memories to function. Given the practical interest of quantum communication — which is often considered the most mature of all future quantum technologies — it is not surprising that the development of quantum memories has become an important and very dynamic field of research.

One of the most advanced approaches is to use a single atom in a cavity. The basic configuration is the same as the one we have seen above. An optical fiber is connected to the cavity. The photonic qubits transported by this fiber can be in two distinct polarization states, which correspond to the two qubit states. When the photon enters the cavity, it is absorbed by the atom with a probability close to one. However, thanks to an appropriate choice of the photon frequency and the atomic species, the atomic state after the absorption depends on the polarization that the photon had. The atom finds itself in one of two possible states, or even in a superposition of the two, depending on the state of the photonic qubit. Thus, the memory function is realized: the photon has disappeared, but the quantum information that it carried is now preserved in the atomic state. The atomic states in question are long-lived states (several seconds and more), more than enough for use in a quantum repeater. To read the memory (*i.e.* to re-emit a photon in the correct polarization state), an additional laser beam is used to excite the atom. It decays by emitting a photon into the cavity. The polarization of the photon depends on the atomic state, thus allowing the original photonic qubit to be recreated.

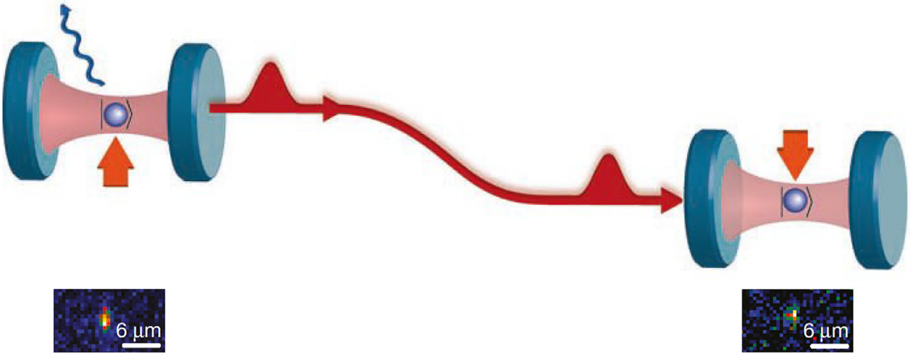

FIG. 3.10 – Elementary quantum network realized in Garching, Germany. The small photograps show the single atoms in each cavity, which form the nodes of the lattice. The two nodes are located in two different laboratories, connected by 60 m of optical fiber. Transverse beams (vertical red arrows) are used to manipulate the state of the atomic qubits and to initiate the state transfer from the first qubit to the second. Unlike a measurement, which projects the qubit into one of the two states $|0\rangle$ and $|1\rangle$, here the full quantum state is transmitted, even when it is a quantum superposition (J. Kimble, CalTech and G. Rempe, MPQ).

Using this approach, a group of researchers from the Max Planck Institute for Quantum Optics in Garching, Germany, have succeeded in combining the transmission, storage and readout of a photonic qubit in one experiment, thus realizing the first elementary quantum network (figure 3.10). This is an encouraging result, even if much remains to be done. For example, the fidelity of the storage — the probability of storing exactly the state of the received qubit and not another one — remains far below its theoretical limit. In the Garching experiment, the main limitation was the weak atom-cavity coupling in the macroscopic Fabry–Perot cavities. Their replacement by FFP cavities is under way.

Advances in cavity technology will improve the coupling, but other approaches also exist. As always in the early days of a new technology, several realization methods are developed in parallel, often cross-fertilizing each other. One interesting approach is to replace the single atom with an ensemble of many atoms. By trapping these atoms inside the volume occupied by the light field, they will absorb the light collectively. The atom-photon coupling is improved: it increases with the square root of the number of atoms. As a trapped atom cloud can easily contain millions of atoms, the coupling can be increased by a factor of a thousand or more compared to the case of a single atom. As long as we can guarantee that there is never more than one photon at the same time (and this is the case in quantum networks), the whole ensemble behaves as a single "superatom", so that we can now envisage a quantum memory without the need for a cavity. However, things get a little more complicated when we take into account the lifetime of this memory. In order to be able to restore the photon correctly at the end of the storage period, each of the atoms must remain at the position it had at the beginning, to within a fraction of the light wavelength. If this is not the case, the partial emissions of the different atoms will not overlap with the correct phase, and the photon will leave in a random direction instead of being emitted into the output mode. If we put all atoms in the ensemble in the same trap, their residual motion limits the lifetime of the memory to a few hundred microseconds at most. Although this may be sufficient in some applications, longer storage is preferable, and can be achieved by confining the atoms in an optical lattice (see chapter 1). Indeed, in such a lattice, the position of each atom is fixed at a specific site, and remains stable to much better than one wavelength during the whole storage period.

A recent experiment carried out by Julien Laurat's team at Laboratoire Kastler Brossel combines these ideas with an efficient and original waveguide, developed a few years earlier by Arno Rauschenbeutel and his team at the University of Vienna. It consists of a stretched optical fiber, tapered to a diameter of 400 nm, (only a few thousandths of its normal diameter) over a length of 1 cm, as shown in figure 3.11. Despite this minuscule diameter, which is only half the wavelength of the light used, the light that propagates in the fiber passes through the thinned region with very little loss: in the LKB experiment, the transmission is 98%. However, the shape of the light mode changes completely in the thinned region. While the light is concentrated in the center of the fiber in the normal regions, a large part of the light field propagates outside the fiber in the thinned region. It forms what is called an evanescent wave at the interface between the glass and the air. By trapping atoms in the immediate vicinity of the thinned fiber (figure 3.11), they couple to the field through this evanescent wave. Although the coupling between an atom and the field is weaker than in a good cavity, the coupling is comparable to that of a good lens (*cf.* figure 3.4),

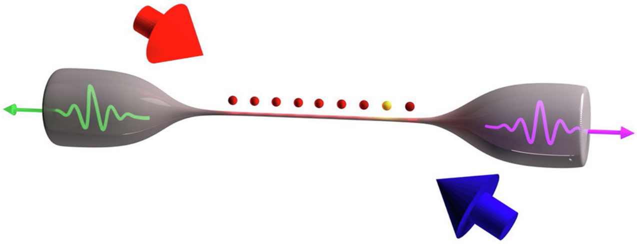

Fig. 3.11 – Schematic of a quantum memory using a tapered fiber and a chain of atoms. In the tapered part, the diameter of the fiber is only 0.4 μm — smaller than the optical wavelength. The atoms, placed in the evanescent field of the tapered fiber, interact with this field while remaining accessible for laser cooling (J. Laurat, LKB).

while presenting several advantages. Unlike the focused field of the lens, the evanescent field of the fiber extends all along the tapered region, allowing a chain of atoms to be placed there as shown in figure 3.11. Furthermore, due to its small diameter, the fiber does not block access to the trapping region, making it much easier to cool and manipulate the atoms. A third advantage is that the light enters and leaves through an optical fiber, as in the FFP cavity seen above. The LKB researchers have demonstrated the storage and retrieval of a photon in this elegant device, establishing it as a promising candidate for the realization of a quantum memory.

These examples highlight the current state of research on cold atom quantum memories. There are still other approaches, where cold atoms are replaced by other quantum emitters. One approach is to use “dopant” atoms implanted at low concentration in a transparent crystal. Owing to the crystal matrix, their positions remain fixed in time, as required for a quantum memory. There is a price to pay, however: the atomic resonances are affected by the presence of the crystal, which broadens and shifts. If these systems are studied as potential quantum memories in spite of this problem, this is because they do not require laser cooling and trapping, which remains relatively complex today. On the other hand, the example of telecommunication optics shows how complex optical systems can be simplified and made robust through clever engineering. A similar development is possible for laser cooling systems. It is quite possible that this development will take place in the years to come, given the increasing number of applications of cold atoms. In any case, research in this field has reached a stage that allows it to evolve from fundamental research to engineering applications.

3.8 Improving Clocks with Entanglement: Spin-Squeezed States

In quantum memories, atoms are an intermediate representation of a quantum state that is photonic before and after. Photons can also be used to create atomic states that are interesting in themselves. This is the case of **spin-squeezed states**, a class of entangled quantum states that have the potential to improve the stability of atomic clocks (see chapter 2). Starting in the 1990s, the potential of these states for metrology was understood, thanks to the theoretical work of the Japanese researchers Masahiro Kitagawa and Masahito Ueda as well as the future Nobel Prize winner David Wineland and his collaborators in the United States. However, at that time, the experimental tools to produce these states were not yet available. Here again, optical cavities have removed a roadblock. Today, spin-squeezed states are a very active field of research, and the realization of the first clocks and atomic sensors enhanced by these states is imminent.

To appreciate the amazing power of these states, we will first briefly consider the role of measurement in a clock or an atomic sensor. The working principle of these devices is explained in chapter 2. Here, it is sufficient to know that the cold atoms in a clock or sensor are in a superposition of two states, $|0\rangle$ and $|1\rangle$, as in quantum information. The measurement that takes place at the end of each clock cycle aims to determine the probability of either state as precisely as possible. However, as we now know, we cannot measure these probabilities directly: during the measurement, each atom is projected into one of the states, either $|0\rangle$ or $|1\rangle$. What we measure is the number of atoms in each of the states, N_0 and N_1. If the probability of the state N_1 is 50%, the difference $N_1 - N_0$ will be close to 0. If this probability increases above 50%, the difference larger and larger positive values. Conversely, the more it falls below 50%, the more negative the difference tends to be. Thus the difference $N_1 - N_0$ measures the probability that we want to know, but it is subject to statistical fluctuations, known in this context by the name of “quantum projection noise”. In spite of this rather pompous name, the situation is exactly that of a simple coin toss, where we want to know if the coin has the same probability for heads and tails. To determine this probability, we will toss the coin a large number of times (or, if we have a large number of identical copies of the coin, we can toss them all at once, just as we use a set of identical atoms in a clock). The result will be subject to statistical fluctuations, which are exactly the same as those of the quantum measurement. Even if the probability of a “head” is exactly one half, it is unlikely to obtain exactly 50 “heads” for 100 trials (figure 3.12). This is why we need to make a large number of trials to reduce this statistical uncertainty: it decreases only with the root of the number of trials, *i.e.*, very slowly. In the atomic case, one might think that we can simply use larger atomic cloud, containing ten or a hundred times more than the hundred thousand atoms of a typical clock today. But this number of atoms is subject to many constraints. It cannot be increased without paying a price, especially in terms of systematic effects. At the beginning of the development of cold-atom clocks, all this was not yet on the agenda: other sources of noise dominated the performance, and quantum projection noise was only a theoretical consideration. But in 1999, after years of continuous improvement, the fountain clock of the SYRTE laboratory at the Paris Observatory was the first to reach this limit. Other clocks followed suit, and researchers remembered spin-squeezed states, which have now become a hot topic. How do these states work, and how can they be produced in the laboratory?

To understand how they work, the starting point is the independence of the atoms in the normal case that we have just described. A given atom’s measurement result is independent of the result obtained for any other atoms. Once again, this is a fact that

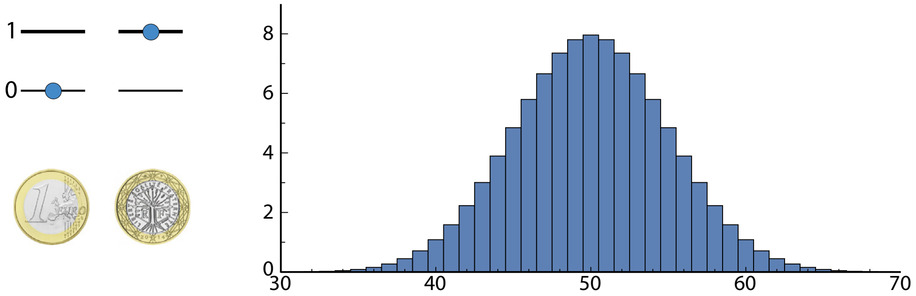

FIG. 3.12 – Frequency of the numbers of atoms measured in the $|1\rangle$ state for a set of 100 atoms, each of which is initially prepared in an equal superposition of the $|0\rangle$ and $|1\rangle$ states. The statistics is exactly the same as for a coin toss repeated 100 times.

we know very well: in spite of what we would like to believe when playing dice, the probability of rolling a 6 never increases, even if we have not had one for many rounds. But, unlike dice, atoms are quantum objects, for which there is a form of correlation that do not exist for classical objects — this is what quantum entanglement is all about. Its most fundamental form is the Bell pair, the perfect correlation between the spins of two particles, made famous by the experiments of Alain Aspect. For a set containing more than two particles, there are many other forms of entanglement. What they all have in common is a correlation between the results when the spins of the particles are measured, whereas each of the spins, taken individually, remains perfectly indeterminate. In the case of spin-squeezed states, the correlation is such that the statistical fluctuations are reduced during the measurement. If, for example, the measurement of the first two atomic spins projects them both into the $|1\rangle$ state, then the probability of finding the third atom in the $|0\rangle$ state increases thanks to the quantum correlation between the atoms. This is how the statistical fluctuations can decrease below the projection noise, if the state of the ensemble is a spin-squeezed state. Nevertheless, for each atom taken individually, both probabilities remain equal to one half, as in a non-squeezed ensemble. We can therefore use the squeezed state in the clock without suffering systematic effects (such as a shift in the clock frequency), and take advantage of the noise reduction in the final measurement.

But how to prepare an atomic ensemble in such a state? The seminal article by Kitagawa and Ueda already proposed a first method. However, it was difficult to apply to clocks, because it involved interactions between atoms, which would disturb clock transition. Once again, atom-light interaction came to help, and CQED methods proved particularly powerful. In a series of papers published in 2010, Vladan Vuletić and his team at MIT demonstrated two methods for producing spin-squeezed states using optical cavities. Several other teams have improved them since. We will describe one of them, which relies on a measurement made by the cavity. The principle is shown in figure 3.13. The atomic ensemble is trapped inside the cavity. As in the qubit detection experiment, three atomic states come into play: the two clock states $|0\rangle$ and $|1\rangle$, separated by a frequency of a few gigahertz (much

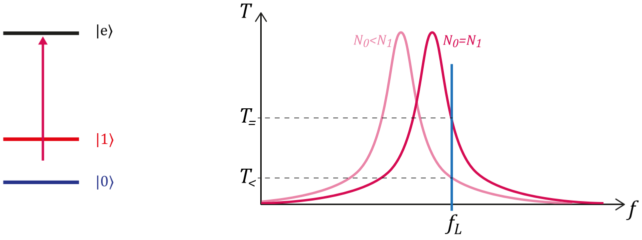

FIG. 3.13 – Principle of the production of a spin-squeezed state by measurement. Left: the atomic ensemble is placed in a cavity; the cavity resonance frequency (red arrow) is detuned at equal distance from the two resonances $|0\rangle$ and $|1\rangle$. Right: when $N_0 = N_1$ (same number of atoms in each of the $|0\rangle$ and $|1\rangle$ states), the cavity frequency is not shifted (dark red curve). When $N_0 < N_1$, it is shifted to a lower frequency (light red curve), and to a higher frequency when $N_0 > N_1$. A probe beam (blue line, frequency f_L) measures this frequency shift. Thus we can determine the value $N_1 - N_0$ without revealing the state of each individual atom.

smaller than an optical frequency) and an excited state, which is linked to each of the clock states by an optical transition. This time, however, the cavity is detuned midway between these transitions. In such a situation, each atom in $|0\rangle$ shifts the resonance in one direction, while each atom in $|1\rangle$ shifts it by the same amount in the other direction: each atom pulls the resonance a bit to its side. Initially, each atom is prepared in an equal superposition of the two clock states. The net result is a resonance frequency that is proportional to the difference in the numbers of atoms in the two states, $N_1 - N_0$. This is exactly the quantity we are interested in. Unlike absorption or fluorescence measurements (which project each atom in one of the two states), here we measure this difference without revealing the state of each individual atom. This is why the measurement projects the atoms into an entangled state, with non-classical correlations: after measurement, we know with good precision the fraction of atoms in each of the states, but the state of each individual atom remains perfectly indeterminate, as required for use in the clock. With a good cavity, a measurement accuracy beyond the projection noise is easily reached.

Figure 3.14 shows a spin squeezing experiment done by Mark Kasevich and his team at Stanford. In this experiment, entanglement reduces the uncertainty on $N_1 - N_0$ by a factor of ten compared to the standard value (the projection noise) in an ensemble of 500 000 rubidium atoms. The principle of the experiment is exactly the one we have just described. To achieve this squeezing value — the best among current experiments — the researchers have developed several experimental tricks, the most important of which concerns the trapping of the atoms in the cavity. The atoms are trapped in a one-dimensional optical lattice formed by a standing wave in the cavity. The cavity is resonant for both the probe beam and the lattice beam. So far, nothing exceptional — the experiments seen above follow the same principle. Here, however, the wavelength of the lattice beam is exactly twice that of the probe beam, so that each lattice site coincides with a maximum of the intensity of the probe beam. This avoids any "blind spot": no atoms escape the probe beam,

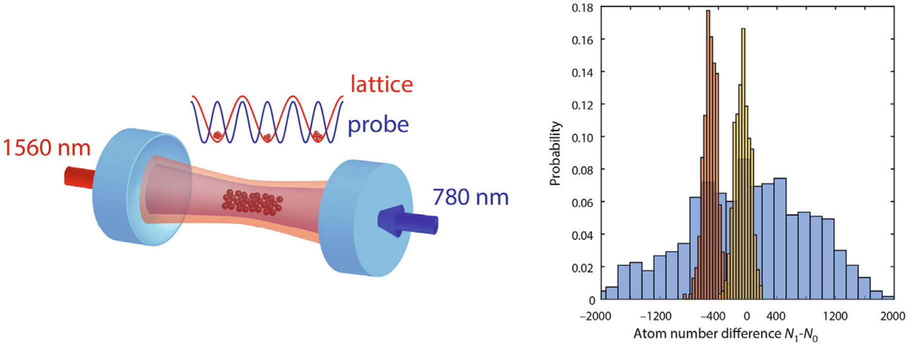

FIG. 3.14 – Results of a cavity measurement of the difference $N_1 - N_0$ of the atom numbers in the two clock states. Left: the atoms are trapped inside the cavity in a first standing wave, which forms an optical lattice (red line). Each lattice site coincides with a maximum of a second standing wave, that of the probe beam (blue line). Thus, all atoms are detected by the probe, there is no blind spot. The principle of the measurement is that of figure 3.13. Right: result of a large number of repetitions of the measurement in different conditions. Each time, a set of 650 000 atoms is prepared in the cavity. For the blue histogram, each atom is prepared in an equal superposition of $|0\rangle$ and $|1\rangle$ states and there is no entanglement between the atoms. In this case, each atom behaves like the coin in figure 3.12 and we obtain the same binomial statistics as in that figure. For the yellow histogram, the spin squeezing procedure is applied before measurement. The fluctuations of the results are much smaller, no measurement deviates from the mean by more than 400 atoms, while the deviation could reach 2000 atoms without spin squeezing. For the orange histogram, the conditions are identical to those of the yellow histogram, but the average value was slightly modified during the preparation: there are 400 atoms less in the state $|1\rangle$. Thanks to the reduced fluctuations of the squeezed state, the difference between the two histograms is clearly visible, while the same difference is drowned in the fluctuations for non-squeezed atoms.

all are maximally coupled. This is a major advantage because a poorly coupled atom is a poorly squeezed atom, which does not participate in the noise reduction. The noise of a few poorly squeezed atoms can be enough to spoil the noise reduction of a much larger ensemble. Here, this problem is eliminated. The noise reduction is immediately visible in the figure: the uncertainty on $N_1 - N_0$ is only 80 atoms, while it is ten times larger for the same ensemble without compression. The entanglement appears here as a resource.

The power of spin-squeezed states being thus experimentally demonstrated, it remains to employ them in real clocks and atomic sensors. Several experiments are underway in Europe and the United States to do just that. Thus, in metrology as well as in quantum information, cold atoms open the way to new applications while pushing further our understanding of the quantum world.

Chapter 4

Quantum Simulation with Cold Atoms

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We have seen in previous chapters how to control with a very high degree of accuracy the position and velocity of an assembly of atoms that can be cooled at extremely low temperatures. Other parameters of the atoms, such as their internal states or their interactions, can also be manipulated. This fantastic degree of control over cold atoms has opened up a very rich set of applications. This chapter deals with the concept of "quantum simulation". The general idea is to take advantage of this extreme control and observation capabilities of cold atoms, so as to experimentally realize "simulators" of systems for which direct computation is out of reach, even with the most powerful computers. For this purpose, the ensemble of cold atoms must be prepared in such a way that they are governed by the same equations as another physical system of interest; these equations are "solved" by its direct physical evolution, and the result is obtained by an experimental measurement made on the atoms.

4.1 What is Quantum Simulation?

4.1.1 From Classical Matter to Quantum Particles

There is a fundamental limit to the precision with which we can simultaneously know the position and the momentum[1] of an object: the better we know the position of a body, the greater the uncertainty about its momentum, and *vice-versa.*

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[1] For a massive particle, its momentum is the product of its mass m by its velocity v.

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This phenomenon, central to the quantum formulation of the laws of physics, is characterized by Heisenberg's uncertainty relation, an inequality which states that the product of the uncertainties on the momentum and on the position of a body is greater than a constant, $\hbar$, called the reduced Planck constant. This fundamental indeterminacy explains why any particle can also behave like a wave, which extends all the more in space the lower the uncertainty on its velocity. This is called a "matter wave". The wavelength called the "de Broglie wavelength", named after the physicist Louis de Broglie who introduced this notion, characterizes the spatial extension of this matter wave (see figure 1.16 of chapter 1). As the momentum of a body is proportional to its mass, the smaller the mass, the greater the uncertainty on the position, the longer the de Broglie wavelength, and the more the particle behaves as a wave. For this reason, it is often said that the wave-like quantum properties of matter are enhanced in the microscopic world. In contrast, the macroscopic world would thus be the realm of classical physics, a classical and somewhat boring world in which "a door has to be open or closed".

However, it would be a mistake to consider that macroscopic objects are entirely governed by the laws of classical physics. Indeed, matter is made up of myriads of microscopic particles, which arrange themselves together, and it is impossible to understand the very stability of matter by ignoring quantum mechanics. For example, any piece of metal is made up of elementary cells, reproduced billions of times identically in all three directions of space in the material, resulting in a crystalline lattice. In this lattice are, at fixed positions, ions characteristic of the material as well as electrons moving more or less freely within the lattice and from one lattice site to another. The average energy E of the electrons is huge: if we expressed it by a fictitious temperature, using the expression $E = k_B T$ (where k_B is Boltzmann's constant), we would find a temperature T higher than 10 000 °C (much higher than the surface temperature of the sun), even for materials at room temperature (20 °C)! This very high energy is explained by another founding principle of quantum mechanics, Pauli's exclusion principle (see figure 1.21 in chapter 1). This principle formalizes the following observation: for a large family of particles (called fermions), it is impossible to find two of these particles in exactly the same state and at the same place. Electrons, like all elementary material particles, are fermions, and therefore obey this "exclusion" principle. As a result, one cannot accumulate a large number of low-energy electrons in a metal, because once the low-energy states are populated by some electrons, other ones can no longer occupy these same states. These electrons therefore have no other "choice" than to occupy higher energy states. In total, the average energy of electrons in a solid is therefore very high. The case of metals (and the most common insulators) is a fascinating example where we can understand the physical properties of macroscopic objects composed of an astronomical number of particles, starting from the quantum properties of their elementary constituents. In this case, the electrical conduction properties ultimately depend only on the number of electrons, and the number of states they can occupy.

Unfortunately, it is generally not possible to account for the properties of materials in this reductionist way. One of the reasons for this is the complexity of the structure of some materials, due to their partially disordered or composite nature. It is also due to the complexity of quantum mechanics, which allows non-local correlations between distant elementary constituents. These non-local correlations cannot be described classically and are referred to as entanglement. To introduce this subtle notion of entanglement we can for example consider a chemical bond between two atoms. This bond comes from the fact that the two atoms share two electrons. Each electron is characterized by an elementary magnetic moment, called “spin”, which is oriented either in one direction or in the opposite one. An electron can therefore be in two states, “up” when the spin is pointing upwards, or “down” if it is pointing downwards. In chemical bonding, whenever an electron is in one state, the neighboring electron is in the opposite state. Thus, even if the orientation of one of the spins is random, their relative (opposite) orientation is completely deterministic. This “link” between the properties of the two electrons constitutes a correlation between the states of two different electrons, which is called “entanglement”. The physicist Erwin Schrödinger was among the first to have realized the very fundamental and astonishing character of these quantum correlations; Albert Einstein spoke of a “spooky action at a distance”, as if the state of one electron controlled that of its neighbor. If the case of two electrons is quite easy to describe, we will see below that a complete description in the case of a large number of electrons is an insurmountable difficulty.

The practical impossibility of understanding the properties of many materials based on the elementary laws of quantum physics is not necessarily a problem in itself. Indeed, it is not necessarily the goal of physics to understand each structure in every detail. Rather, the objective that can be set is to determine a certain number of general laws, a certain number of principles that govern the organization of matter. However, over the XXth century, the study of the properties of materials, particularly of some materials at low temperatures, has kept challenging the researchers, to the point that a unified understanding is still lacking at the present time.

4.1.2 Challenges in Understanding Complex Quantum Systems

One of the most fascinating discoveries has been that of superconductivity, which occurs for some metals at very low temperatures (see figure 4.1). In 1911, Heike Kamerlingh Onnes discovered that mercury becomes a perfect conductor below a temperature of about 4 K, *i.e.* 4 degrees above absolute zero, which is at −273 °C. Those metals characterized by a strictly zero electrical resistance are called superconductors. They are particularly interesting materials because they allow the transport of strong electrical currents (and for example the creation of strong magnetic fields) without loss of energy. This phenomenon of superconductivity has been explained by one of the most remarkable theories elaborated in the 20th century, the BCS theory of superconductivity, from the initials of its inventors John Bardeen, Leon Cooper and John Schrieffer, who were awarded the Nobel Prize in Physics in 1972. This is another instance of a theory that explains (about 50 years after the experimental discovery of superconductivity) a confusing property of macroscopic materials thanks to the laws of quantum mechanics! The electrical resistance of the material vanishes because the electrons pair up to form pairs that propagate without dissipation in a wave-like manner. To understand this

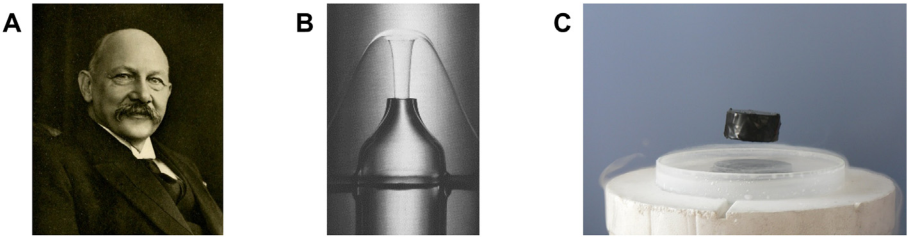

Fig. 4.1 – (A) Heike Kamerlingh Onnes (1853–1916) was the first physicist to cool helium to liquefaction temperature. He was awarded the Nobel Prize in Physics in 1913 for his work on cryogenics. (B) At low temperatures, liquid helium becomes *superfluid*: it loses all viscosity and flows without resistance, giving rise to unusual phenomena, such as the fountain effect shown here. (C) Similarly, at sufficiently low temperatures, some materials become *superconducting*: their electrical resistance strictly vanishes. A magnet placed on a superconductor can levitate above the superconductor. These phenomena have forged our understanding of the physics of collective effects of quantum origin. But other phenomena, now observed for 35 years, remain mysterious, such as superconductivity at a high critical temperature.

phenomenon, we rely on another discovery of quantum physics: two associated fermions no longer behave like a fermion, but like another type of particle, a “boson”, which has radically different properties. Bosons are the second large family of particles allowed by quantum mechanics after fermions. Unlike fermions, bosons “like” to be in the same state (see figure 1.21 in chapter 1). Paired electrons are thus bosons, and the waves describing each of these composite bosons “like” to propagate at the same time in the same direction. They thus can carry an intense electric current without the dissipation usually associated with electrical resistance.

Some more recent experimental discoveries do not fulfill this ideal dream of physicists where each astonishing observation ends up finding its clear explanation. For instance, the discovery of high-temperature superconducting materials has been a source of great frustration. These materials, which nothing seemed to predispose to favorable conduction properties, are superconducting at such high temperatures that they fall outside the validity of the BCS theory! More recently, other materials, superconducting or not, have further complicated the picture, and a unified description of the exotic conduction properties of these materials is still being sought. The challenge lies not only in the fundamental interest of understanding original properties, but also in the possible application of these new systems for information storage (especially quantum information) or energy transport. Indeed, unfortunately, the temperature at which some of these materials become superconducting (typically below −100 °C) is still too low for important applications in industry and energy transport. It would be ideal to engineer new superconducting materials that would operate at room temperature…

But why are these new exotic systems so difficult to understand? There is good reason to believe that the properties of the elementary constituents of these materials, and in particular those of the charge carriers, the electrons, are marked by strong quantum correlations. These so-called “strongly correlated systems” are in principle extremely difficult to describe from a theoretical point of view. To understand this difficulty, let us recall that each electron can be in one or the other of two states, called "up" or "down". If you consider N electrons, each of which can be up or down, the number of states that are accessible to this system is equal to 2^N. If you try to compute, for example, the number of potentially accessible states for an assembly of 300 electrons (which corresponds approximately to the number of electrons in a tiny piece of solid of just 1 nm^3), you will find a number that is far beyond the number of atoms contained in the Universe (see figure 4.2)... This estimate shows that we cannot hope to describe exactly the state of electrons in a highly correlated quantum system such as those in which high-temperature superconductivity occurs.

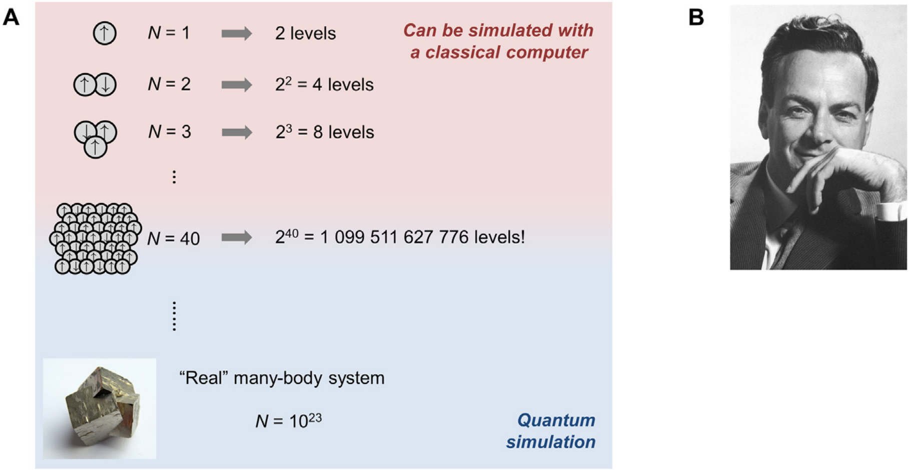

FIG. 4.2 – The complexity of a many-body system is gigantic if all possible microscopic configurations are taken into account. (A) Even for an elementary two-state constituent such as a spin 1/2 (the simplest quantum system), the complexity of the mathematical problem to be solved to study the behavior of a system of N particles increases very rapidly (like 2^N) with the size of the system. The best current supercomputers can, at best, solve the dynamics of about 40 spins, while a real system has about 10^{23} constituents! (B) Richard Feynman (1918–1988, Nobel Prize in Physics 1965) suggested in 1982 the concept of quantum simulation to tackle this kind of problems.

Over the last thirty years or so, plenty of approximate models tried to account for the surprising transport properties of highly correlated electronic materials, and those of high-temperature superconductors in particular. But no consensus has yet been reached. The difficulty is quite fundamental: to describe these materials, we have to make approximations; but, how can we be sure that these approximations are relevant? In the end, as long as we do not understand the most confusing properties of quantum mechanics such as entanglement, can we hope that an approximate description will meet with consensus?

Over the past decade, a novel approach has been explored, in particular by the cold-atom research community. This approach takes up a visionary idea of the famous American physicist Richard Feynman (figure 4.2), who suggested to use a well-controlled quantum system to mimic another quantum system. This idea of quantum simulation, which is the subject of this chapter, is the following: let us build a quantum system atom by atom, as perfectly isolated from the environment as possible. Let us put each atom in a perfectly chosen location. Let us control the way these atoms interact with each other. We will thus build a perfectly determined quantum system; and the study of its properties will show whether this system shares some of the surprising properties of highly-correlated electron systems. Sounds like a crazy dream? Many people have already embarked on the adventure!

4.2 Ultracold Atoms and Quantum Simulation

4.2.1 Ultracold Gases: Dilute Systems with Complex Collective Behavior

Quantum gases, which we thus seek to transform into “quantum simulators”, are assemblies of atoms in a very cold gas phase. Thanks to magnetic fields or lasers, these atoms are confined in immaterial “traps”, within sealed containers where a very high vacuum is made, and they can therefore be considered as systems that are perfectly isolated from their environment. They are very dilute, about a hundred million times more dilute than a liquid for example, or about a hundred thousand times than ambient air. Their specificity lies in their extremely low temperature, close to absolute zero; therefore, the de Broglie wavelength, which characterizes the spatial extension of matter waves, can be greater than the average distance between atoms in the gas. In this regime, atomic waves interfere with each other. The consequence of these interferences depends on the quantum nature of the particles forming the cold cloud (see figure 1.21 of chapter 1). If the particles are fermions, the atoms avoid sharing the same wave function (due to Pauli’s exclusion principle, introduced above), the interference is destructive, and the atoms then form a Fermi sea where all lower energy states are populated — this state is similar to the state of electrons in metals at room temperature described at the beginning of the chapter. While for the other family of particles, namely bosons, the interference is instead constructive, and the atoms form a “Bose–Einstein condensate”, named after the physicists Satyendranath Bose and Albert Einstein who predicted its existence, and where all atoms are described by the same wave — this state is similar to that of a laser where all photons share the same mode.

Thus, we see that gases of sufficiently cold atoms can show collective behaviors (similar to those of lasers for bosons or to those of electrons in solids for fermions), simply because of their quantum nature. Because of the interference between atomic waves, cold gases behave like macroscopic quantum objects, characterized by a kind of overall cohesion, even when the interactions between atoms can be considered as negligible.

The most interesting collective behaviors of ultra-cold gases, and the most relevant for quantum simulation issues, nevertheless come from interactions between atoms. When the interactions are attractive, the cloud contracts as it can lower its energy by shrinking; this phenomenon leads to a collapse of the cloud in the case of Bose–Einstein condensates (see figure 1.20 of the chapter 1). When atoms are confined in a trap with a specific geometry (in particular when the trap is very confining in two directions of space so that the cloud has a very elongated shape), this collapse can be avoided and stable clouds can be obtained. These structures do not collapse because the attraction between atoms is compensated by a kind of quantum pressure, which comes, once again, from Heisenberg's uncertainty relations: the reduction in the size introduces an uncertainty in momentum, associated with a kinetic energy, which tends to oppose the collapse. These stable, localized, and non-dispersing structures have been called solitons, in reference to solitary hydrodynamic waves observed under certain conditions in channels, or light solitons observed in optical fibers (see figure 4.3B).

When the interaction between atoms is repulsive, on the contrary, ultracold gases are intrinsically stable. In the case of condensates, the interactions between atoms reduce the compressibility of the cloud, and make it stable even when it propagates; the propagation is then done without dissipation, *i.e.* the cloud is superfluid, in the same way as liquid helium at very low temperatures (see figures 4.1B and 4.3B).

Finally, interactions between atoms can depend on their internal state, *i.e.* on the orientation of their spin. In this case, the magnetic properties of clouds of cold atoms can be studied, and they have striking analogies with magnetic properties in solids (see figure 4.3C).

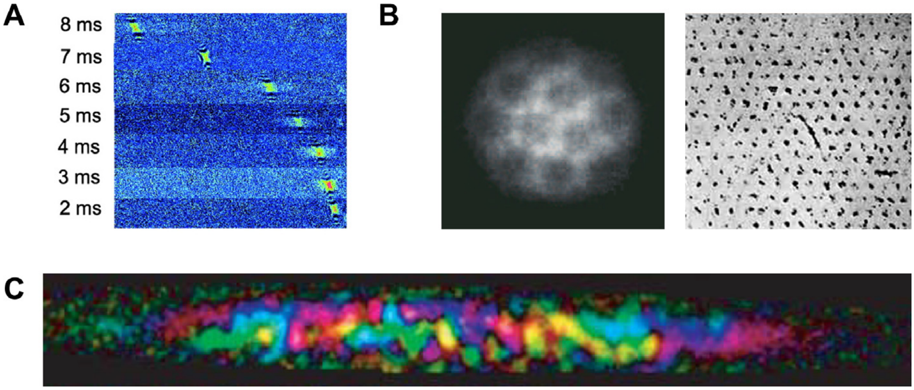

FIG. 4.3 – Quantum gases can have collective properties similar to those of condensed-matter systems. (A) A soliton, obtained with a Bose–Einstein condensate presenting attractive interactions, is a matter wavepacket that propagates without deforming, unlike a gas without interactions (figure reproduced with the permission of Christophe Salomon). (B) A vortex lattice in a rotating quantum gas, revealing its superfluid character (left, figure courtesy of Jean Dalibard), very similar to the *Abrikosov lattice* observed in type II superconductors (right). (C) False-color image of magnetic domains inside a condensate having several spin states, similar to the Weiss domains of a ferromagnetic material (figure courtesy of Dan Stamper–Kurn).

Solitons, superfluidity, magnetism... The study of cold atoms naturally leads to an exploration of collective effects in quantum systems, and these effects have very close links with those observed in very different fields of research: condensed-matter physics, laser physics, non-linear systems (see figure 4.3). Research in the field of cold atoms has thus greatly benefited from past and present advances in other fields: observations carried out on cold atoms have led to the "rediscovery" of collective phenomena already described for other systems. However, these "rediscoveries" benefit from a very different experimental context, which often brings new insights, and in particular allows finding a particularly simple microscopic explanation to macroscopic phenomena. After having been guided so well by the previous discoveries of condensed-matter physicists, is it possible that in the near future, research on cold atoms leads to a better understanding of the still poorly understood macroscopic quantum phenomena arising in other fields? This is the question opened by the concept of quantum simulation with cold atoms.

4.2.2 Why are Cold Atoms Good Quantum Simulators?

Here we will try to identify, from a practical point of view, what makes cold atoms so promising in the context of quantum simulation.

First of all, two atoms of the same atomic species and in the same internal state are indistinguishable. These are quantum objects whose internal complexity can be high (each atom being made up of tens of interacting electrons, protons and neutrons), but which are characterized by very well defined internal states, and identical for all atoms of the same species. For example, two rubidium atoms can be prepared in exactly the same quantum state by simple experimental methods. This fundamental property is one of the most striking interests of cold atoms, compared to more macroscopic quantum objects (quantum dots, superconducting qubits), which are not perfect copies of each other, and therefore are intrinsically distinguishable.

The indistinguishability of atoms is also guaranteed because atoms can be deterministically trapped in extremely well-controlled potential wells; these potentials are made "by hand" using electric and magnetic fields, and can be identical in several positions in space. This differs strongly, for example, from the case of "color centers", one of the most widely used systems in quantum information (a field of research directly related to that of quantum simulation). In that case, the aim is to probe the spin of particles located in a crystal, which then see a potential fluctuating according to their local environment in the crystal. In contrast, the atoms, trapped in vacuum, are protected from such uncontrolled fluctuations, and thus constitute a clean quantum system that is very well isolated from the environment.

An additional advantage of cold atoms is that one can produce quite "macroscopic" samples in terms of particle number. While cold ions (other excellent candidates for quantum simulation) can be trapped in tens or perhaps hundreds, atoms are trapped in hundreds of thousands. This large number of atoms gives access to a gigantic number of configurations, which is an important criterion for quantum simulation.

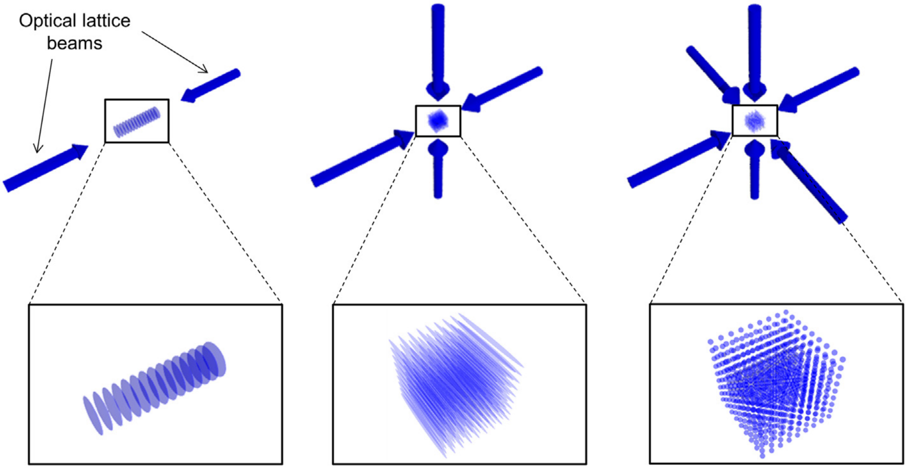

FIG. 4.4 – An optical lattice is the dipole potential obtained by interfering several laser beams. Depending on the number of beams that are used, we can obtain one-dimensional arrays of discs (left), two-dimensional arrays of tubes (middle), or three-dimensional arrays of spherical wells (right).

A particularly interesting system is realized by optical lattices, introduced in chapter 1 (figure 4.4). They are obtained by superimposing laser beams on the atoms. The standing wave produced by the interference of the laser beams produces an almost ideal periodic potential in which the atoms are trapped. The minima of the potential form the "sites" of this periodic lattice. The atoms can move in this lattice by jumping randomly from one site to a neighboring site (this is called the tunnel effect, another entirely quantum effect). And when they occupy the same site, they collide and interact. The result of this game of love and chance is to generate quantum phases that are very interesting from the point of view of the quantum simulation of magnetism. For instance, we can work in a regime where each site of a three-dimensional lattice contains one and only one atom. Physicists study such systems because they realize arrays of localized spins, which are at the basis of our understanding of magnetism.

Other methods, which will be described below, also make it possible to trap samples of atoms, one by one, in optical tweezers whose position can be controlled very precisely. This approach makes it possible to study many-body systems in a bottom-up approach, starting from just a few atoms and adding them one by one.

Finally, as noted above, the very rich phenomenology of many-body systems is governed by the interactions between particles. One of the fascinating properties of cold atoms is that one can control the interactions between them. Atoms are neutral particles, since the positive charge of the atomic nucleus is compensated by the negative charge of the electrons. Therefore, in a first approximation, we can consider that the electrostatic interactions cancel out at large distance. However, when two atoms approach each other at a distance which is not very large compared to their size, they become sensitive to the distribution of charges around the nucleus. Long before the electron orbitals of two atoms overlap, *i.e.* at distances of several tens of nanometers, the atoms feel the presence of their partners, and interact through a so-called van der Waals interaction that comes from the fluctuations in the position of the electrons around the nuclei. One of the beauties of atomic physics is that this interaction can in fact be controlled by subjecting the atoms to a magnetic field (figure 4.5A). In this way, during a collision between two atoms, they can be made to bind briefly to form a molecule. By adequately choosing the value of the magnetic field, the conditions for atomic binding are more or less met, so that the effective interaction energy can be tuned (figure 4.5). We speak of Feshbach resonances (from the name of Herman Feshbach, who described similar processes for neutron physics) to describe this process (also mentioned in chapters 1 and 7) where two atoms briefly bind to form a molecule. The strength of the interaction can be controlled over several orders of magnitude, and the interaction can be made attractive or repulsive.

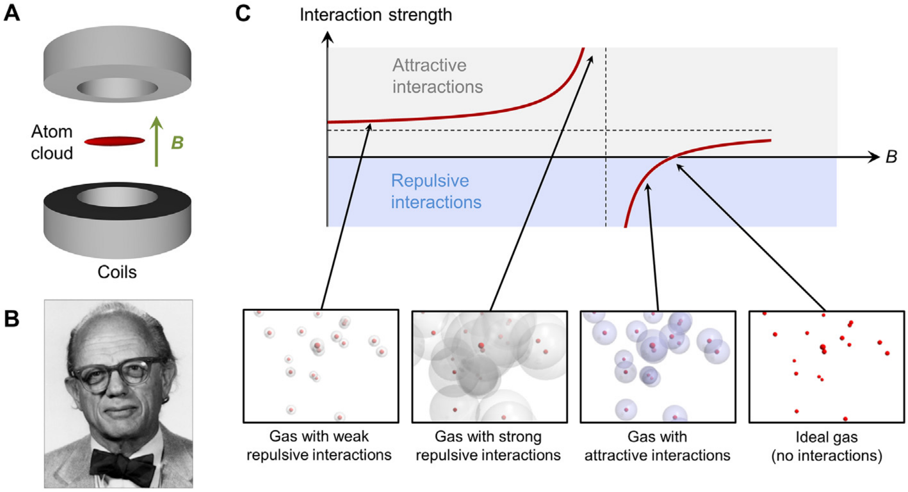

FIG. 4.5 – Using coils through which an electric current flows, a controlled magnetic field of strength B can be applied to a cloud of atoms (A). This makes it possible, using a so-called "Feshbach resonance", in reference to the American physicist Herman Feshbach (1917–2000) (B), to control the strength of the interactions between atoms: (C) depending on the applied field, the interactions can be weak or strong, attractive or repulsive, and can even vanish.

This control of interactions, which, as stated above, are at the microscopic origin of the macroscopic quantum phenomena that we are trying to understand better, is one of the most remarkable assets of cold atoms. Let us take an example, which has been explored in many laboratories around the world. For these experiments, the atoms we consider are fermions. A mixture of atoms in two different spin states is placed in a trap. The energy of interaction between the atoms is varied. If the interaction is attractive, we obtain a system of fermions that attract each other weakly, and the system has strong analogies with the above-mentioned superconductors described by the BCS theory. If the interaction is repulsive, on the contrary, a completely new superfluid system can be created: a condensate of atom paired into molecules. The interaction energy can also be arbitrarily increased, and a maximum so-called "unitary" interaction regime is reached, which allows to reproduce in the laboratory the interaction conditions that are encountered in neutron stars!

As we can see, the control of interactions makes the field of application of cold atoms very vast. Especially since we can also consider changing the very nature of interactions between atoms. Indeed, van der Waals interactions, which are only felt at small distances between atoms, can be "replaced" by longer range interactions when the atoms have a sufficiently large magnetic moment. In this case the atoms can interact in a way similar to that of two magnets interacting with each other. These interactions are called "dipolar" interactions. Needless to say, this type of interaction between cold atoms is particularly interesting for the study of magnetism, which is precisely the study of the interaction between magnets! Another way to have strong and adjustable dipolar interactions between atoms is to excite them to so-called "Rydberg states", very close to the ionization threshold. These correspond, in a classical picture, to atomic states where an electron orbits around the ion core of the atom on a trajectory which is very large at the atomic scale, which gives them a very strong electric dipole moment. These states have a finite but very long lifetime, and two atoms prepared in this way can interact very strongly by the electric dipole–dipole interaction. We will come back to this in section 4.3.2.

4.3 Observing a Quantum System Atom by Atom

The main characteristics that make cold atoms interesting from the point of view of quantum simulation have been described above: they are isolated macroscopic systems with a large number of particles, whose interactions and motion can be carefully controlled. However, a physical system is only really interesting and useful if one knows how to make precise measurements on it: the art of a physicist is that of measurement.

It is from the point of view of measurement that some of the most impressive experimental developments in the field of cold atoms have recently occurred (see chapter 2). Here, we will describe in more detail two experimental systems that are very interesting from this point of view.

4.3.1 Visualizing Atoms in an Optical Lattice

A first approach, which emerged about ten years ago, is based on the realization of quantum gas microscopes (figure 4.6). This approach consists in loading ultra-cold atoms in a two-dimensional optical lattice, and then observing the fluorescence light emitted by the two-dimensional array of atoms thus obtained (see figure 4.6A). To do this, we use a high numerical aperture optical microscope objective. In practice, the resolution can be better than one micrometer. In this way, one can detect the

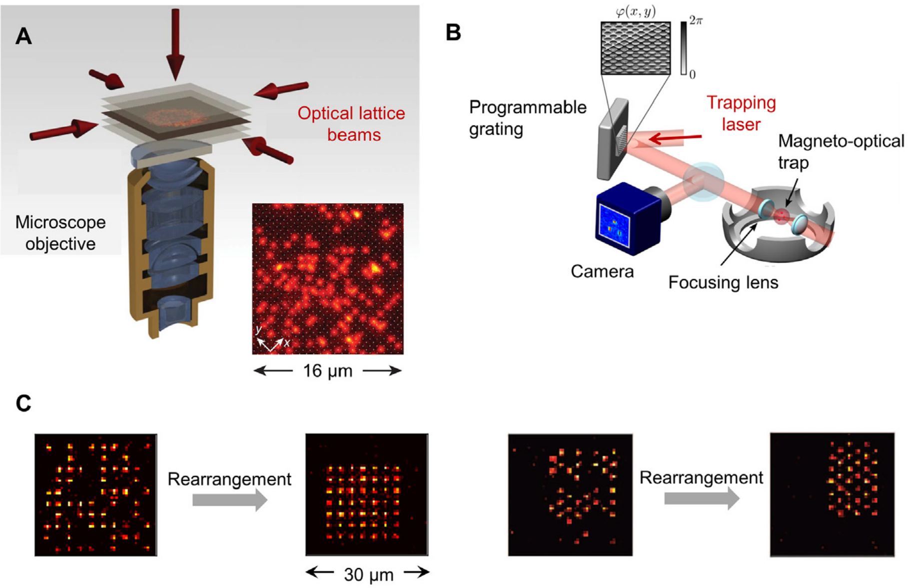

FIG. 4.6 – One can observe an atom cloud trapped in a periodic potential with single atom resolution. (A) In a *quantum gas microscope*, a microscope objective is used to observe the fluorescence emitted by atoms trapped in an *optical lattice* (see figure 4.4). The inset shows the image obtained when a Bose–Einstein condensate is loaded in the array. Each bright dot corresponds to a single atom. Figure reproduced with the permission of Stefan Kuhr. (B) Another approach is to use *optical tweezer arrays*. A highly focused laser beam inside a magneto-optical trap is used to trap one and only one atom, and a computer-programmed diffraction grating is used to create an array of such tweezers. (C) The initial array is randomly loaded with a 50% loading probability for each trap; using computer-controlled moving optical tweezers, the atoms are actively reorganized to obtain a regular square or triangular array.

atoms individually, distinguishing in which site of the array they are located, and thus, in a way, "take a picture" of the state of the many-body system. Using a mixture of atoms populating two spin states, several teams have recently demonstrated the appearance of an antiferromagnetic order at low temperatures. The system then spontaneously organizes in a spatial configuration where the spins of the atoms point alternatively in one direction and in the opposite direction, from one site of the lattice to the next (see below, in particular figure 4.7C).

4.3.2 Assembling Artificial Crystals Atom by Atom

In quantum gas microscopes, we start from a large number of atoms (several hundred thousand) but finally keep only a few hundred at most. Recently, this so-called top-down approach has been challenged by a bottom-up approach, where one directly controls the atoms one by one, and gradually increases the size of the system. The basic ingredient is the trapping of individual atoms in optical tweezers (figure 4.6B–C). These are simply focused laser beams, as in the case of the optical tweezers mentioned in chapter 1, but this time on a size of the order of a micrometer. These form microtraps in which previously laser-cooled atoms can be confined, at temperatures of a few tens of microkelvins above absolute zero. The tiny size of the trap means that when a second atom enters the trap, the two atoms are lost almost instantaneously due to two-body losses induced by the presence of light: one of the two atoms absorbs a photon, and the two atoms are then violently attracted to each other, giving them such a high energy that they are ejected from the trap. A source of single atoms is thus realized: an optical tweezer cannot contain more than one atom (but it can also, with the same probability, be empty). The presence of the atom can be optically detected by the light it scatters. In order to study many-body physics, one starts by creating a large number of optical tweezers by holographic techniques using a computer-controlled diffraction grating, which makes it possible to arbitrarily choose the spatial arrangement of the tweezers (see figure 4.6B). However, as each microtrap is randomly occupied by only 0 or 1 atom, one obtains disordered spatial configurations of atoms, which change from one repetition of the experiment to the next. To solve this problem, the atoms are reorganized by moving them, using a moving optical tweezer, thus creating regular arrays of atoms separated by a few micrometers (see figure 4.6C). At this distance, the atoms in their ground state hardly interact at all; to turn on interactions between atoms, they are excited to Rydberg states using lasers, which allows very strong interactions that affect the internal degrees of freedom of the atoms. This makes it an ideal system for the quantum simulation of magnetism, with in particular a very large freedom in the geometrical arrangement of the atoms: one can switch from a square lattice to a triangular geometry (figure 4.6C) with just a few mouse clicks!

4.4 What can We Simulate with Cold Atoms?

4.4.1 Quantum Magnetism

The use of the systems described above initiated the exploration of strongly correlated quantum systems with cold atoms. The birth of this type of research was the observation in 2001, in Immanuel Bloch's group in Germany, of the phase transition between a superfluid state and a "Mott insulator" when a Bose–Einstein condensate is placed in an optical lattice. This transition is obtained by simply varying the laser intensity that produces the optical lattice, *i.e.* by varying the depth of the potential wells.

This state has been named in analogy with some insulating states introduced by Nevill Mott (figure 4.7) in the context of solid-state physics. A usual insulator is a solid where electrons cannot circulate freely because of Pauli's exclusion principle: for each given spin state, one electron exactly populates each site of the solid crystal lattice, which prevents any other electron of the same spin state from circulating, because two identical electrons cannot occupy the same position. We then have exactly two electrons in each site of the crystal, one for each of the two possible spin states. A Mott insulator is a particular insulator in which there is exactly one electron only at each site of the crystal lattice, but each electron can then be in one of the two permitted spin states. In principle, the electrons could circulate freely because the Pauli principle does not prevent two electrons with different spins from occupying the same position; however, the repulsion by the Coulomb electrostatic interaction between the two electrons is so strong that it prevents them from occupying the same site. As a result, the system becomes insulating. In a Mott insulator, it is thus the electric repulsion between atoms (Coulomb blockade) that prevents transport.

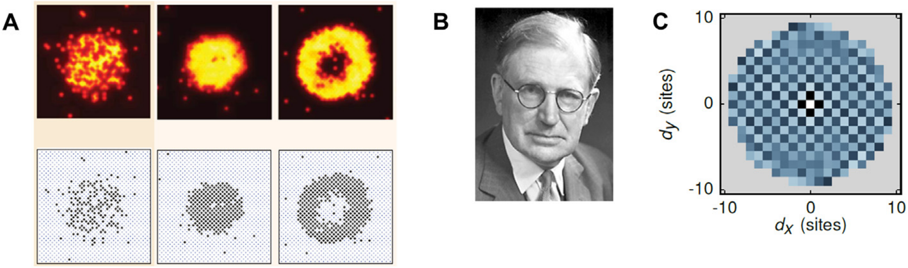

FIG. 4.7 – Cold atoms reproduce some of the emblematic phases of strongly correlated electron physics. (A) Phase transition between a superfluid and a Mott insulator, observed with a quantum gas microscope. The lower images are obtained by digital processing of the raw images (top); a black dot indicates the presence of an odd number of atoms at each site of the lattice. In the superfluid phase (left) the number of atoms per site fluctuates strongly; in the insulating phase, the number of atoms per site is fixed (one in the middle column; two in the center and one in the periphery for the right column). Figure reproduced with the permission of Stefan Kuhr. (B) Nevill Mott (1905–1996), the British physicist who introduced the metal–insulator transition that now bears his name (Nobel Prize in Physics 1977). (C) The Néel antiferromagnetic order (see text) is observed directly with a fermionic quantum gas microscope (figure reproduced with the permission of Markus Greiner). The orientation of the spins alternates from one site to another. There is good reason to believe that the study of this system in the presence of "holes" will teach us something about high-temperature superconductivity.

With cold atoms, an analogous insulating state is obtained when a repulsive interaction energy exists between the atoms (figure 4.7). It is this type of state that was observed for the first time in the experiment mentioned above. Mott insulators first introduced in the physics of strongly correlated electrons thus also exist in the realm of cold atoms. These observations again illustrate the fertile analogies explored by this field of research, and the potential of these systems as quantum simulators. It also exemplifies the new possibilities opened by research with cold atoms, since the Mott state created in these experiments is a Mott state with bosonic particles, in contrast to the case of electrons (which are fermions as we have seen). The case of bosons is very different from that of fermions, because the conductive state, obtained when the optical lattice is shallow, is superfluid. By simply increasing the laser intensity that produces the lattice, we change the ability of atoms to jump from one site to the next by tunneling, and we observe a sudden change in transport properties, which characterizes a phase transition between a superfluid state and an insulating state.

As shown in figure 4.7A, the Mott transition with cold atoms can be observed with single atom sensitivity using a microscope that visualizes the lattice sites one by one. At low lattice depth, we see that the number of atoms fluctuates from one lattice site to another, a necessary condition for the appearance of superfluidity. On the contrary, for deep lattices, the atoms are "blocked", with one atom per lattice site, and cannot move. We have a Mott insulator.

The Mott insulator with cold fermionic atoms was produced a little later, and characterized under an optical microscope. Here again, cold atoms demonstrate both their ability to visualize a strongly correlated state atom by atom, and to provide a microscopic characterization of states first introduced in the context of solid-state physics. But there are other possibilities: for example, using ytterbium atoms, a Mott state has been produced with fermions which, instead of having just two spin states (up and down) like electrons, have up to six. Thus, we obtain new highly correlated systems with novel and interesting properties.

4.4.2 Origin of Superconductivity

Recently, research has focused on the cooling of Mott states to temperatures where not only is there exactly one atom per site, but also, a magnetic order arises. Indeed, at very low temperatures, a magnetic transition occurs: when the temperature is low enough, we observe that the spins arrange themselves spatially in the lattice so that they point alternately up and down. This phase transition, called "Néel's transition", has been observed by directly measuring the spin orientation of the atoms at each site of a lattice. We then observe a kind of checkerboard pattern, where the black squares represent an atom whose spin is pointing up, and the white squares represent an atom in the down state (figure 4.7C).

By cooling more and more the spins in the lattice, we expect to get closer and closer to the ground state of this interacting spin system, where the macroscopic spin of the assembly of atoms is globally zero. It is a particularly interesting state from the point of view of quantum simulation. Indeed, if this state is well understood from a theoretical point of view, we cannot predict what happens when we add "holes" in such a system (*i.e.* when we "simply" remove atoms). The success of such an experiment would be particularly interesting, by the analogy it brings to the poorly understood physics of high-temperature superconductors. Indeed, experimental observations indicate that the superconducting state arises when holes are added to a magnetically ordered state similar to the Néel state. Would studying a similar situation with cold atoms also allow a better understanding of the physics of high-temperature superconductors? If so, this would undoubtedly be a successful demonstration of the power of the quantum simulator approach, since a detailed understanding of high-temperature superconductivity is still elusive at this time.

4.4.3 Improving our Understanding of Strongly Correlated Materials

If we try to summarize the interest of cold atoms for quantum simulation, we can say the following: we are exploring physical phenomena that have very strong analogies with some effects that occur in complex physical systems, for which quantum correlations complicate theoretical simulations; and these phenomena can now be studied with new tools, the ones described above. The systems we use are practically isolated from the environment; one can control the motion and interactions between particles; one can measure the state of the atoms one by one; and the time scales involved allow one to observe, with the same ease, stationary states and states that evolve over time. Furthermore, we have also pointed out that atoms have an internal structure (resulting from the association of their numerous nucleons — protons and neutrons — and electrons) that can be used to broaden the field of research. This is the case, for example, of magnetism: if electrons have only two possible spin values, corresponding to an “up” or “down” orientation, some atoms have a higher complexity in their ground state: this is the case of the strontium atom with its ten possible spin states in the ground electronic state.

These possibilities make cold atoms excellent quantum simulators. What they allow is not just to make more precise studies: observing a many-body system atom by atom, studying its time evolution, measuring either the speed or the position of particles. It is also possible to create new types of states: taking advantage of the fact that atoms have a spin greater than that of electrons, introducing a coupling between the spin of atoms and their motion, so as to create artificial magnetic fields much higher than those to which electrons can be exposed. Thanks to these new possibilities, it should be possible to accumulate experimental observations of various many-body quantum systems that had been inaccessible until now. As a result, these studies help putting research on many-body quantum systems in a broader framework, in order to discover general trends that they follow and to improve our understanding of these systems.

For instance, consider the case of fermions located in optical lattices. By performing experiments, we should be able to test whether the system becomes superfluid at low temperatures in the presence of holes (initially empty sites), which would demonstrate a phenomenological link with high-temperature superconductivity. We will also be able to characterize the quantum entanglement or correlations that arise in these types of superconducting materials, we will be able to know if superconductivity survives if, instead of having two populated spin states, we have three, four or more, we will be able to know how this type of system evolves as a function of time.

Thus, a quantum simulator built with cold atoms can be expected to bring a better understanding of the physics of materials with strong quantum correlations, and to allow a more global understanding of many-body physics. It should also be noted that experimental advances and new tools specific to cold atoms represent new challenges from the point of view of theoretical physics: since we know how to measure differently, this leads to the development of new protocols, new theoretical tools, for example to describe the dynamics, the collective properties when there is a large number of possible spin states… It is also simply a matter of deciding which observation is relevant; indeed, it is not possible to measure all the interatomic correlations for a large number of atoms, and it is therefore necessary to decide what is useful to measure. Recent research on the physics of many-body quantum systems with cold atoms has led to the creation of new states, which have collective quantum behaviors that need to be characterized. New "entanglement witnesses" are being sought, *i.e.* measurement protocols that could be used to directly demonstrate the appearance of quantum correlations, or even to quantify them and refine the understanding of their nature. To do this, one must be able to take advantage of the new possibilities offered by atoms. This is a good example of a back and forth exchange between theory and experiment, showing how new experimental tools help create new concepts, and how these can in turn influence experimental research.

4.4.4 Other Prospects

We end up this chapter with a non-exhaustive list of topics that are currently being addressed by cold-atom physicists in the hope of realizing quantum simulators. This chapter has dealt extensively with the case of magnetism and superconductivity, which is an emblematic but not unique case. Let us also mention frustrated quantum systems: these are states that have many accessible magnetic configurations at low energy, which has important consequences on the obtained magnetic phases. Other research has focused on strongly interacting gaseous fermionic systems, and has led to experiments that are relevant to a better understanding of the physics of neutron stars. Some researchers also use cold atoms to better understand electronic transport problems in the quantum regime. The question of transport in the presence of disorder is developed in detail in chapter 5. We also study the dynamical evolution of systems placed in an excited state, and we try to better understand in which case a quantum system can relax towards equilibrium, and in which case, on the contrary, it can remain "trapped" far away from its equilibrium state.

These studies are related to open problems in mathematical physics, and are linked to fundamental questions of thermodynamics, in particular those dealing with the articulation between the thermodynamic laws of macroscopic systems and the underlying microscopic laws, of a quantum nature. Analogies with other fields of physics also sometimes arise because of symmetries and associated conservation laws. Thus, by studying atoms that can present three equivalent spin states, we can address some questions related to the physics of quarks, these elementary constituents of nucleons, which also occur in three different forms. Similarly, when four spin states are accessible, it is with graphene physics that some experimental results can be compared. From quarks to neutron stars, from thermodynamics to the

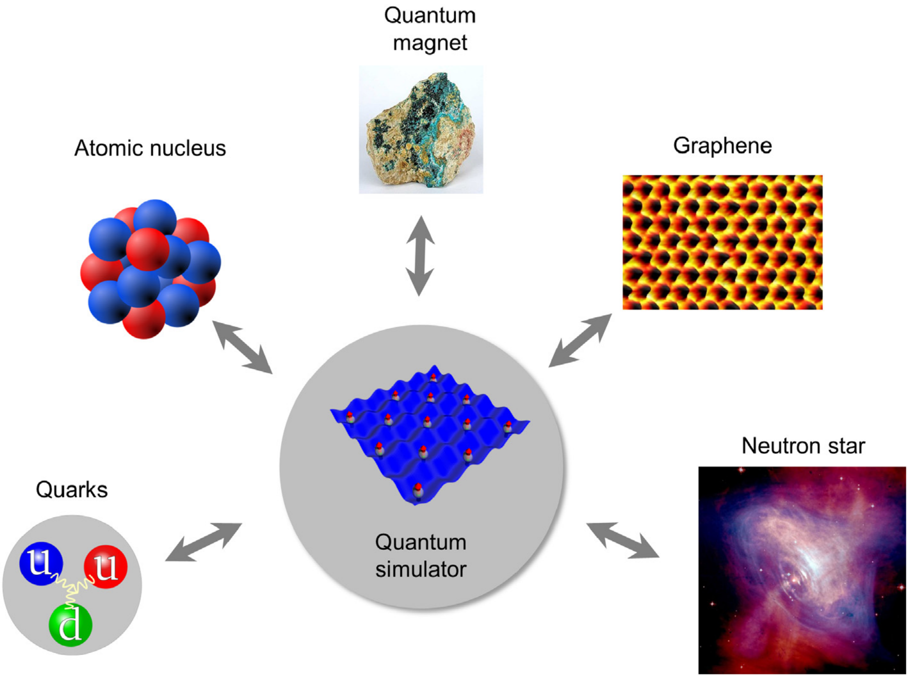

Fig. 4.8 – Quantum simulation with cold atoms makes it possible to explore a very wide variety of physical phenomena, usually encountered in fields as diverse as particle physics (quarks), nuclear physics (atomic nucleus), solid-state physics (magnets, graphene), astrophysics (neutron stars), etc.

infinitely small, physicists interested in the concept of quantum simulation seek to link their studies to a wide variety of fields (figure 4.8). The ambition may seem excessive, but it is perhaps also the expression of a simple conviction: the laws of nature are the same everywhere. Let us hope that this postulate continues to be as fruitful as ever!

Chapter 5

Waves and Disorder

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In close connection with the use of cold atoms as "quantum simulators", which is the subject of chapter 4, a new branch of atomic physics has developed in recent years: the study of matter waves in the presence of disorder. A spectacular phenomenon of disordered systems is Anderson localization, named after its discovery in 1958. It predicts that the interference between multiple scattering paths of a de Broglie wave may stop its propagation, thus transforming a conducting material into an insulator! Motivated by the remaining open questions around this emblematic phenomenon, the physics of cold atoms in the presence of disorder has been naturally focused, from the beginning, on the possibility of studying experimentally Anderson localization. This problem will therefore be extensively discussed in this chapter. More generally though, the complexity associated with multiple scattering of waves in disorder gives rise to a wide variety of physical phenomena, which go much beyond Anderson localization. We will end this chapter by giving an overview of these phenomena and the associated questions, especially in the case of interacting systems.

5.1 Waves and Disorder, very Rich Physical Systems!

5.1.1 Diffusion in Disorder: an Intuitive Approach ...

Disorder is omnipresent in our environment, so that situations involving the propagation of a wave in a disordered medium are not lacking! We can think of light waves in clouds, acoustic and elastic waves in biological tissues, or electronic de

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Broglie waves in conducting materials (see figure 5.1a). Whether the waves are classical or quantum, the physical description of their propagation is identical: one decomposes it into successive changes of the trajectory on the obstacles, which are for example the water droplets in suspension in the cloud, or the impurities of the conductor in figure 5.1a. In the case where interferences between the different trajectories are negligible, this process of successive collisions is similar to a "simple" random walk of a purely classical particle. As illustrated in figure 5.1b, the typical distance explored after time t is then:

$$\Delta r_{\text{diffusive}} \simeq \sqrt{2D_0 t} \tag{5.1}$$

where D_0 is the diffusion coefficient, of the order of vl^*, with v the velocity of propagation of the wave and l^* the average distance between two changes of trajectory, called the transport mean free path. This intuitive approach in terms of classical particle diffusion is relevant to describe many propagation phenomena. It is, in particular, at the heart of the radiative transfer theory of classical waves, or of the Drude model for electronic conduction.

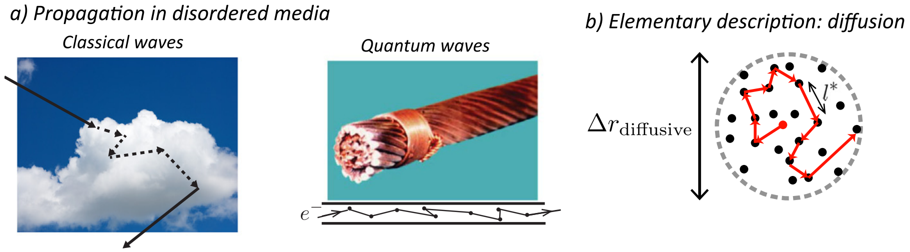


FIG. 5.1 – (a) Two physical situations involving the propagation of waves in a disordered medium. A classical wave, the light, whose trajectory is deviated by water droplets in a cloud, and a quantum wave, an electron evolving in a conductor presenting defects. (b) Illustration of propagation in terms of successive scattering events, separated by an average distance l^*, the transport mean free path. This description, where interference effects are neglected, corresponds to a diffusive random walk. After time t, the wave explores a region of size $\Delta r_{\text{diffusive}}$, where D_0 is the diffusive coefficient, see equation (5.1).

5.1.2 ... Which Hides a Much More Complex Physics!

There are, nevertheless, situations where the diffusive model does not allow to correctly describe observations. A first reason is due to interferences between trajectories. These can have a significant impact, especially when the waves travel along "loops" as we will see in section 5.3. The extreme case is Anderson localization, a regime where the propagation is completely stopped, and which will be extensively studied in the following. Without going that far, interferences in disorder are at the origin of various phenomena, referred to as *weak localization* effects, whose study was historically at the origin of the development of mesoscopic physics in the 1980s. These phenomena are, for example, the negative magneto-resistance observed in conducting films, or the mechanism of coherent backscattering which will be discussed in section 5.4.

Interferences are, however, not the only cause of the complex behavior observed in certain disordered systems. For quantum waves, interactions between particles – for example Coulombian interactions between electrons – also have dramatic effects! In general, it is the subtle interdependence between the processes of diffusion, interference and interactions that makes the physics of disordered systems extremely rich. The phenomena resulting from this interplay are very diverse, ranging from metal–insulator transitions – or even superfluid-insulator transitions such as the Mott transition described in chapter 4 –, to the thermalization of quantum systems.

5.1.3 A Physics also Source of Innovation

In this chapter, we will concentrate on the fundamental aspects of the research on disordered systems with cold atoms, trying to give the simplest possible intuitive picture. However, we should mention that a whole area of research in this field is also dedicated to applications. The idea is no longer to consider disorder as a nuisance, but to take advantage of it in order to develop innovative applications. Giving an exhaustive list of the explored tracks would be too long here, and it is not the object of this chapter, but let us mention the possibility of imaging or focusing through opaque media – with important applications for biomedical imaging –, or to improve the efficiency of photovoltaic sensors or light-emitting diodes.

5.2 Cold Atoms: Disorder Under Control!

5.2.1 How to Immerse Atoms in Disorder?

Understanding the physics of disordered systems requires experiments in which the statistical properties of the disorder are perfectly controlled. This is, indeed, an essential condition if one wants to validate or invalidate the theoretical models that are developed to account for observations. In many situations, however, it is difficult to know exactly what the disorder is. It is often even naturally present, as for impurities in electronic materials. As we will see in this section, cold atom systems allow for a precise control of the disorder applied to the atoms. For this reason, they constitute nearly ideal platforms for studying the physics of disorder, in line with the research aiming at realizing quantum simulators.

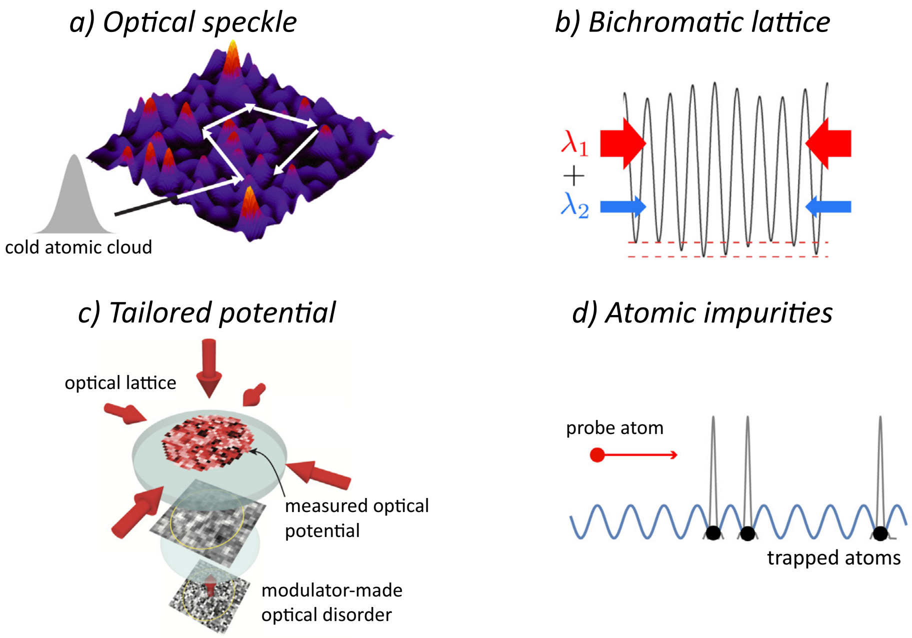
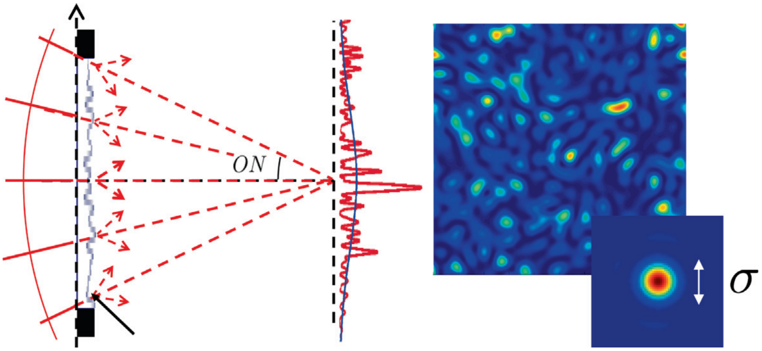


Fig. 5.2 – Examples of disordered potentials for cold atoms. (a) Laser speckle disorder. (b) Bichromatic lattice resulting from the superposition of two optical lattices of slightly different wavelengths. (c) Potential resulting from the superposition of a tailored optical disorder created with a spatial light modulator and a main optical lattice (from Choi *et al.*, *Science* **352**, 1547, 2016). (d) Disorder created by scattering on randomly located atoms.

Different methods have been developed to create disorder for atoms, some examples being shown in figure 5.2. Among them, two have been especially used, in particular during the first experiments on Anderson localization in 2008 (see section 5.3.3): the laser speckle and the bichromatic lattice. In both cases, one uses the fact that the disordered potential is directly proportional to the light intensity, as in the case of the optical traps presented in chapter 1. The speckle field is obtained by diffraction of a laser beam on a rough plate, yielding a completely random intensity pattern (see box 5.1). The bichromatic lattice uses the combination of two optical lattices at two different wavelengths, one being of low amplitude and playing the role of a quasi-random modulation of the main lattice. While these types of disorder are the most common, other methods are currently being developed. It is, indeed, also possible to use spatial light modulators, similar to what can be found in video-projectors, allowing to project directly on the atoms a predetermined light distribution (see figure 5.2c). With this method, used in particular in the many-body localization experiments that will be described in section 5.6.2, one no longer controls only the global statistical properties of the disorder, but the precise value of the disordered potential at each point in space.

Box 5.1: The laser speckle, a "natural" disorder for cold atoms



Diffraction by a roughened glass plate

speckle «grain»

An optical speckle is created by the diffraction of a laser beam on a rough plate. This plate induces a random phase that varies at each point such that the diffraction pattern can be interpreted in terms of random multi-wave interference. Visually, the random illumination is composed of grains of light more or less intense, isolated from each other by areas where the intensity is almost zero. Depending on whether the laser is blue or red detuned (see chapter 1), these grains act as potential wells or bumps for the atoms. It can be shown that the characteristic grain size of the speckle (which can be rigorously defined by the correlation function, see bottom right inset), corresponds to the diffraction limit:

$$\sigma \simeq \frac{\lambda}{2\mathrm{ON}} \sim 0.5\,\mu\mathrm{m}, \tag{5.2}$$

i.e., the smallest achievable size for a given ON numerical aperture.

The common feature between the disorders presented above is that they are all created using random intensity patterns of light that are imaged on the atoms. As a result, all these potentials have a typical length scale of variation – called the correlation length and usually denoted σ, see box 5.1 – which is at least as large as the diffraction limit of the optical system. This characteristic size, of the order of a micrometer, plays a crucial role because it defines a typical energy, and thus a temperature, below which the interesting quantum phenomena will occur. Precisely, quantum effects will be revealed if the de Broglie length λ_{dB} of the atoms, as introduced in chapter 1, is greater than or equal to σ. Since λ_{dB} is related to the velocity of the atoms and thus to their temperature, one can estimate the maximum temperature below which the quantum effects become important:

$$\lambda_{dB} \gtrsim \sigma \Rightarrow T_{\mathrm{typ}} \lesssim \frac{1}{k_B}\frac{\hbar^2}{m\sigma^2} \simeq \text{a few nanokelvins.} \tag{5.3}$$

The study of quantum transport therefore requires extremely low temperatures! One understands why it is necessary to start from ultra-cold atoms, typically a Bose Einstein condensate, in the experiments that will be described hereafter. Let us note, finally, that we have listed here the most common situation where the realized disorder varies randomly in *space*. There is, however, another configuration, just as interesting, where the potential varies in time and not in space. The physics associated with this "temporal disorder" will be discussed in section 5.5.3.

5.2.2 Random Walk of Cold Atoms in Disorder: Observation of Diffusion

Achieved in the mid-2000s, the ability to observe Anderson localization in the controlled disordered potentials described above has triggered a new line of research for cold atoms. Before coming back to this "quest for localization" in the next section, let us first address a natural question, although historically explored lately: is it possible to observe the "simple" diffusive behavior of cold atoms in disorder, as expected for classical particles (see figure 5.1b)?

To answer this question, let us distance ourselves a little from the chronology by discussing first the experiment shown in figure 5.3a, performed in 2010 at the Charles Fabry laboratory. In this experiment, a cloud of cold rubidium atoms is prepared in an optical trap to serve as a "source point". The experiment starts by switching off the optical trap while switching on another laser propagating horizontally, very focused in the vertical direction but extended in the transverse, horizontal directions, so as to realize a kind of "light sheet" which confines the atoms in a horizontal plane. In the absence of disorder, the atomic cloud expands ballistically: the size Δr of the cloud evolves proportionally to time t, in both directions of the plane. The typical surface $S(t)$ on which the atomic cloud extends thus varies as the square of the time: $S(t) \propto \Delta r^2 \propto t^2$. The number of atoms N being constant, one can easily imagine that the atomic density at the center of the cloud, $n(t) \sim N/S(t)$, will decrease as $1/t^2$, as shown in figure 5.3b.

If we repeat the same experiment but, this time, in the presence of disorder, the behavior is of course different. Indeed, the atoms now evolve following a multiple scattering process similar to a random walk (see section 5.1). In this case, the expected spreading is diffusive, according to equation (5.1), so that the density at the center of the cloud now behaves as:

$$n(t) \propto 1/\Delta r^2_{\text{diffusive}} \propto 1/t. \tag{5.4}$$

As shown in figure 5.3b, this $1/t$ decay law, *i.e.*, a direct signature of atomic diffusion, is exactly the one observed in the experiment! Note that to observe this diffusive motion, the researchers have increased the temperature of the atoms in order to inhibit, on purpose, the effects of quantum interference at the origin of the famous Anderson localization, on which we will now focus.

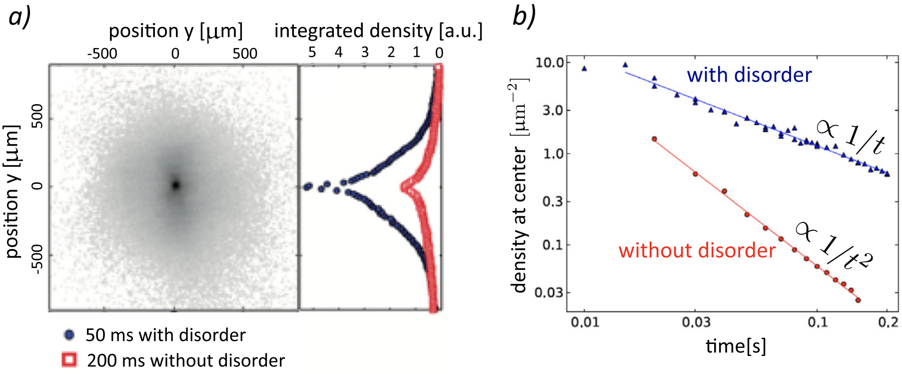


Fig. 5.3 – Classical diffusion of cold atoms in a speckle disorder, from M. Robert-de-Saint-Vincent *et al.*, *Phys. Rev. Lett.* **104**, 220602, 2010. (a) Fluorescence imaging of a rubidium atomic cloud after expansion in the presence of disorder. The profiles along the y direction correspond to two successive expansion times. (b) Evolution of the atomic density at the center of the cloud as a function of time t, with or without disorder. The $1/t$ decay is a direct signature of the diffusive behavior.

5.3 Anderson Localization: Halted by Disorder

5.3.1 60 Years of Investigations and Still Open Questions

To understand the continuing interest in Anderson localization, it is useful to begin by briefly describing the history of this phenomenon. It was discovered in 1958 by Philip Anderson (see figure 5.4), who realized that conduction in metals could be completely stopped in the presence of sufficiently strong disorder. In dimension three, Anderson localization even leads to a quantum phase transition: above a certain critical energy electrons are able to propagate, while at low energy transport is suppressed and the conductor becomes an insulator. This discovery was revolutionary at the time, because it completely challenged Drude's classical view of electronic transport. However, it did not draw a lot of attention until the 1970s, where a simple and elegant phenomenological description was proposed, known today as the *scaling theory of localization* and based on the pioneering work by David Thouless (see figure 5.4). The scaling theory, in addition to unifying Drude's and Anderson's views of transport in metals, also provides general predictions about the Anderson localization phenomenon and, in particular, emphasizes the role of the spatial dimension, points that we detail in section 5.3.2. In the wake of these theoretical results, several experiments have demonstrated the halt of electronic transport due to disorder in metals. Figure 5.5a illustrates this phenomenon in a disordered alloy: at sufficiently low temperatures, the conductivity of the metal cancels out and the material becomes insulating.

At the same time, physicists quickly realized that the localization phenomenon was an interferential mechanism. With this picture in mind, it is clear that it is not

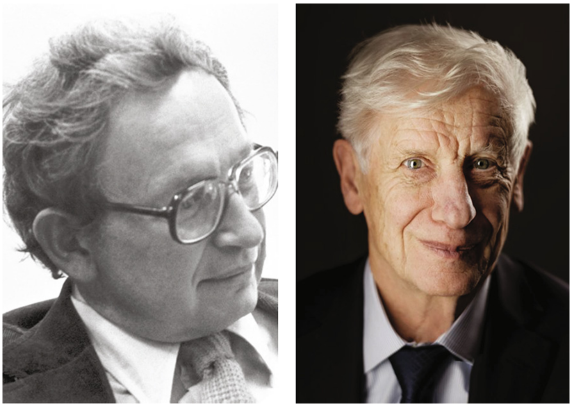


FIG. 5.4 – Philip Anderson (left) and David Thouless (right), both Nobel laureates. Credit: *nobelprize.org*.

specific to electrons but exists for any type of wave, whether it is of quantum or classical nature. Thus, since the 1990s, several experiments reported the localization of classical waves such as light or elastic waves, especially in one (1D) and two dimensions (2D), see figure 5.5b and c for some examples. Note that the question of localization of light in three dimensions (3D) remains open at the moment, as the Anderson phase transition has not yet been clearly observed in optics, see the discussion in section 5.5.

Generally speaking, the study of the Anderson transition in 3D remains an important issue in the field. No exact theory capable of quantitatively describing this transition has been established to date. Therefore, many questions remain open, such as the possibility to predict precisely the critical energy E_c of the transition, called the *mobility edge*. Even more fundamental is the determination of the critical exponent of the transition. This critical exponent characterizes the behavior of transport properties near the mobility edge, such as the way the diffusion coefficient cancels out when approaching the transition from the diffusive side. Similarly, this exponent describes how the localization length – which we will introduce in the next section – evolves as one approaches the mobility threshold from the localized side. The fundamental interest for this critical exponent comes from the fact that it does not depend on the specificities of a given disordered system: its value is *universal*, *i.e.*, it is the same whatever the type of wave or disorder considered! Theoretically, this value has only been determined by numerical simulations. On the experimental side, only one experiment – using an analogue of Anderson localization based on temporal disorder and presented in section 5.5.3 – has been able to measure it precisely.

Before turning to the experiments carried out in recent years in the field of cold atoms, we will first discuss a little more in detail the physics of Anderson localization in order to propose an intuitive understanding. This will be the occasion to emphasize the essential role played by the dimension on the localization properties.

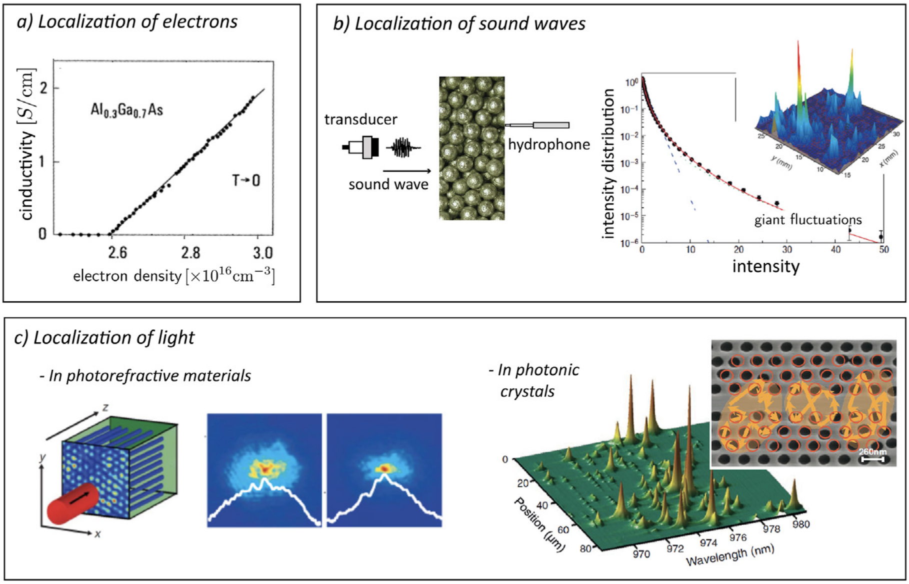


Fig. 5.5 – Some landmark experimental observations of Anderson localization. (a) Localization of electrons in metals (adapted from Katsumoto *et al.*, *J. Phys. Soc. Jpn* **56**, 2259, 1987). At sufficiently low temperatures, a metal can become insulating because of the disorder. Here one approaches the transition to the insulator by decreasing the density of free electrons. For a certain critical density, the conductivity cancels out. (b) Localization of acoustic waves (from Hu *et al.*, *Nature Physics* **4**, 945, 2008). Here, a sound wave propagates through a disordered array of aluminum spheres. The spatial intensity distribution is measured at the output with a hydrophone. This distribution decreases slowly, indicating giant fluctuations in intensity, characteristic of waves localized by disorder. (c) Localization of light. On the left, in a photorefractive crystal made of a disordered array of waveguides (from Schwartz *et al.*, *Nature* **446**, 52, 2007). A light beam sent into the medium diffuses transversally at low disorder (left profile), and localizes at high disorder (right profile). On the right, observation of one-dimensional localized modes in a disordered photonic waveguide (from Sapienza *et al.*, *Science* **327**, 1352, 2010).

To finish this general introduction, let us stress that Anderson localization is a *single particle effect* purely related to disorder. The case of interacting atoms, more complicated, will be addressed at the end of the chapter.

5.3.2 An Intuitive Understanding of Anderson Localization

As mentioned above, Anderson localization is a complex phenomenon, which has given rise to an enormous amount of theoretical work aimed at understanding its underlying mechanisms. Without going too much into the details, we can get a first intuitive idea by considering a particular type of interference mechanism where the wave returns to its starting point after having propagated along a "loop" in two opposite directions. As explained in box 5.2, this type of process, which is beyond classical diffusion, increases the probability for the wave to return to its starting point, thus preventing it from propagating over large distances. This mechanism leads to a decrease in diffusion coefficient D with respect to its classical value D_0.

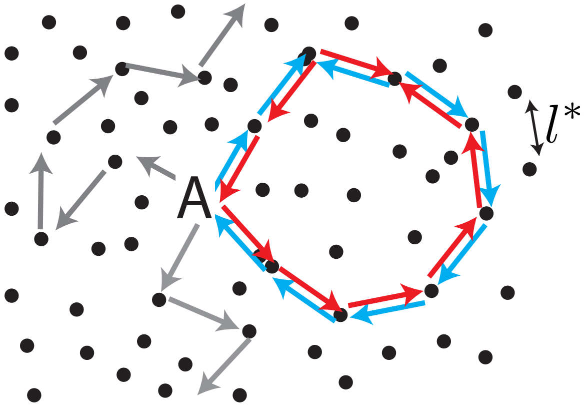
Such kind of interferences along loops are known as *weak localization* effects, and are considered as precursors of Anderson localization. Taken only one by one, they do not lead directly to the total suppression of transport: the diffusion coefficient is indeed decreased ($D < D_0$) but it does not cancel *a priori*. It is the accumulation of these processes that can drastically impact transport and give rise to Anderson localization that corresponds to $D = 0$. To understand this, let us consider the impact of the decrease of the diffusion coefficient on the "weight" (or occurrence) of weak localization processes. Indeed, if the diffusion coefficient decreases, the wave will propagate less easily, *i.e.*, it will remain closer to its starting point. The probability of making loops, as illustrated in box 5.2, will therefore increase, which will further strengthen weak localization processes! A decrease of the diffusion coefficient thus gives rise to a further decrease of this coefficient, and so on... It is this "snowball effect" that eventually leads to the complete cancellation of diffusion. In terms of propagation, this means that the wave freezes around its starting point: Δr stops growing after a certain time and remains constant. An emblematic signature of the Anderson localization is then the exponential decrease of the wave function as a function of the distance to the origin, according to:

$$\psi(r) \propto e^{-|r|/l_{\text{loc}}}, \tag{5.5}$$

where the characteristic decay length l_{loc} is called the *localization length*.

The interpretation of Anderson localization in terms of interference on loops remains an oversimplified picture, because other, more complex mechanisms may also be at work. Besides its simplicity, however, this picture has another advantage: it allows to get an intuitive idea of the crucial role played by the dimension on the localization properties. Indeed, one understands from the previous discussion that the efficiency of the localization processes is directly related to the weight (or occurrence), negligible or not, of the loops compared to the set of possible trajectories. In one dimension, these processes are dominant, since at each reflection on a scatterer, the wave is sent back on its steps. In two dimensions, the weight of the loops – related to the probability of returning to the starting position – is strongly reduced but remains non-negligible in general. In dimension three, the weight of the loops is even less important and becomes negligible, except in the case of strong or even extreme disorder, as discussed in section 5.3.4.

Box 5.2: How interferences prevent wave propagation



Consider the situation where a wave is emitted at point A and propagates as a random walk. As discussed in section 5.1, the classical approach consists in neglecting interferences between the different paths, the propagation being then globally diffusive. Indeed, the accumulated phase along each path depends very strongly on the precise spatial arrangement of the scatterers. On average, we therefore expect interferences to vanish very quickly.

What is true for most trajectories, however, is not true in the particular case where the wave follows a loop (red trajectory), *i.e.* it returns to the initial point after a certain number of scattering events. If the wave propagates one way, the reciprocal path (blue trajectory), for which the wave follows the same path but in opposite direction, also exists. The phase accumulated by the wave on these two paths being identical, the interference is therefore constructive at point A, and this constructive interference will survive an averaging over disorder. Such loops double the probability to return to the origin compared to a classical random walk: *interference thus favors the localization of the wave around the emission point*. In practice, this mechanism reduces the diffusion coefficient D from its classical value: $D < D_0$.

From these considerations, one can guess that localization processes are *a priori* very efficient in 1D, less important in 2D, and almost negligible in 3D. Mathematically, this intuition has been validated by the scaling theory mentioned in the previous section: in 1D and 2D one can show that all wave functions are localized – even though the localization length l_{loc} becomes exponentially large in 2D –, while in 3D there is a phase transition between a diffusive behavior at weak disorder, and localization at extreme disorder.

5.3.3 Anderson Localization of Cold Atoms: First Observations

The experimental quest for Anderson localization of cold atoms has been the driving force of this research field since the mid-2000s. Indeed, although the physics of Anderson localization has been known for more than 60 years, no experiment had so far been able to directly observe this phenomenon for matter waves. After first unsuccessful attempts, which we will not mention here but which were very important to identify the adequate experimental conditions, the first direct observation of the Anderson localization was realized in 2008 at the Charles Fabry laboratory (see figure 5.6).

In this experiment, the configuration was one-dimensional, a situation for which the localization phenomenon is particularly spectacular. Indeed, the localization processes being very efficient in 1D, Anderson localization can be observed even for a very weak disorder. One can then realize a situation where the energy of the atoms is much higher than the disordered potential, so that they "fly" above the disorder without any possibility of being trapped classically (see figure 5.6a). An analogy of this configuration would be a golf ball flying over the grass, the blades of grass constituting the fluctuations of the potential. In this classical picture, we know that nothing can stop the atoms! However, when they are cooled to very low temperatures (see condition 5.3), the quantum reflections on the barriers of the potential are exacerbated, and, as predicted by Anderson, these quantum reflections "join forces" together to stop the propagation. The wave function is then localized, with an exponential decay following the expression (5.5).

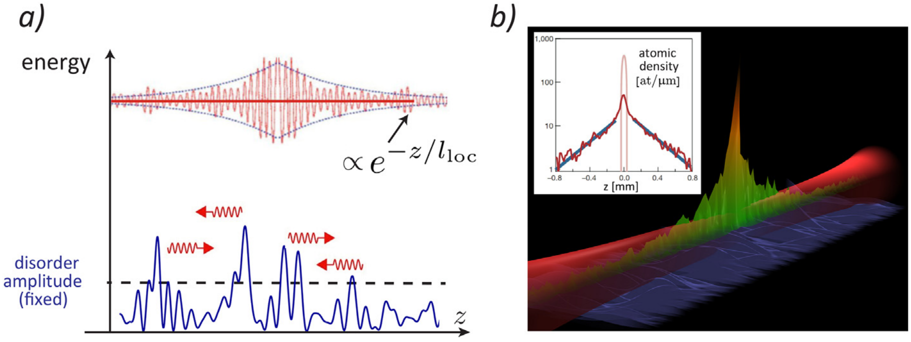


Fig. 5.6 – Observation of Anderson localization of cold atoms in 1D. (a) In the configuration of the experiment, the atoms "fly" above the disorder, *i.e.*, their energy is much higher than the amplitude of the disorder. The typical wave function of a localized atom, whose envelope decreases exponentially, is represented in red. It is superimposed onto the disordered potential, represented in blue. (b) Graphical representation of the atomic density of the localized wave function (in green) in the laser speckle disorder (in blue). The atoms are confined in an optical guide (whose trapping potential is visible in red) and can only move in one direction. The inset shows the atomic density measured by fluorescence imaging in semi-logarithmic scale: the wings indeed decay exponentially in space.

The scheme of the experiment performed in 2008 is very similar to the one previously discussed for the study of classical diffusion: one observes the expansion of a cloud of ultra-cold atoms – which serves as a source point – in the presence of a disorder realized from a laser speckle. In order to make them evolve in 1D, the atoms are guided in one direction by a red detuned laser beam (see chapter 1). The amplitude of the disorder is chosen to be very small, in order to make sure that it is impossible to explain a possible halt of the expansion by a simple classical trapping in the maxima of the potential. And yet, after a certain time of expansion, the atomic cloud freezes! The precise study of the atomic density profile, observed directly by fluorescence imaging, reveals the expected exponential decay (see figure 5.6b), *i.e.*, the emblematic signature of Anderson localization. Cherry on the cake: the localization lengths extracted from the observed decays are in very good agreement with the theoretical predictions, without any adjustable parameter!

This experiment, as well as another one based upon a similar principle and carried out at the LENS (European Laboratory for Non-Linear Spectroscopy) in Florence, Italy, had an important impact in the field of ultra-cold atoms. Indeed, beyond the historical importance (first direct observation of Anderson localization with matter waves), these experiments have demonstrated the relevance of the study of disordered systems with atoms, extending the concept of quantum simulation to another domain. From then on, the research turned to various problems related to disorder. These include, in particular, the effect of disorder in interacting systems, which will be discussed at the end of this chapter, and also, of course, the possibility of studying the Anderson transition in 3D.

5.3.4 Towards the Study of the Anderson Transition in 3D

The difficulties of studying the three-dimensional Anderson transition, which are both theoretical and experimental, lie in the fact that the transition occurs for extremely strong disorder. Indeed, as discussed previously, in general the weak localization processes along loops (see box 5.2) have, in 3D, a negligible weight compared to the set of possible trajectories. In order to increase this weight, the intensity of the disorder must be strongly increased so as to force the wave to remain close to its emission point. The extreme case is reached when mean transport path l^*, defined in paragraph 5.1, becomes of the order of the de Broglie wavelength λ_{dB}. This condition is called the *Ioffe-Regel criterion*, which is usually written as:

$$kl^* \simeq 1 \quad \text{Ioffe-Regel criterion} \tag{5.6}$$

with $k = 2\pi/\lambda_{dB}$ the wave number. It is broadly accepted that this criterion gives the order of magnitude of the position of the Anderson transition (the mobility edge), which is illustrated in figure 5.7. Another intuitive way to understand this criterion is to realize that the quantity kl^* corresponds to the typical phase shift accumulated between two successive scattering events of the wave on the disorder. When the Ioffe-Regel criterion is verified, the phase shift of a backscattered wave on an obstacle is necessarily in phase with the incident wave: the constructive interference to stay around the initial position is then strongly amplified, leading to the localization phenomenon.

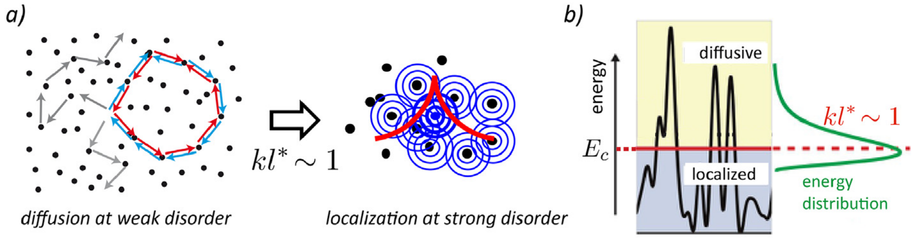


Fig. 5.7 – (a) Anderson transition in 3D. At weak disorder the behavior of the wave is diffusive with possibly a few weak localization loops, and the propagation can be described by a succession of scattering events. At strong disorder, the wave is localized. As the wave has no time to make a single oscillation before being scattered again, the interferences (represented by the blue circles) are strongly enhanced. The transition between the two regimes is characterized by the Ioffe-Regel criterion $kl^* \simeq 1$, equation (5.6). (b) Energy diagram showing the critical energy E_c of the transition (the "mobility edge", represented in red) corresponding to the Ioffe-Regel criterion in the case of a fixed disorder amplitude (the fluctuations of the disordered potential along one direction are represented by the black curve). The green curve shows the energy distribution of the atoms in the presence of disorder. This distribution is strongly broadened by the disorder when it becomes intense enough to reach the Ioffe-Regel criterion. As discussed in the text, this energy broadening is currently the main obstacle to accurately study the transition.

From a theoretical point of view, it is very complicated to describe the propagation properties in this regime of extreme disorder where the wave barely has time to perform an oscillation before being scattered again. One thus understands why developing a quantitative theory of the Anderson transition remains a current challenge. But the difficulties encountered to study the transition are not just theoretical! Experimentally, a major challenge is to keep a precise control on the parameters of the system in the limit of a strong disorder. For light waves, for example, it is very difficult to create strongly scattering media without avoiding the appearance of absorption or non-linear effects, both of which can hide or even destroy localization phenomena.

It is with a clear awareness of these difficulties that different teams have embarked on the study of the transition in 3D with cold atoms. We will not give much detail here about the technical developments that were necessary to go from a one-dimensional to a three-dimensional configuration. These include the implementation of a magnetic levitation system to prevent the atoms from falling under the effect of gravity, and the use of the most isotropic optical disorder possible by crossing different speckles (see figure 5.8). Apart from these complications, the principle remains the same: a cloud of ultra-cold atoms is released in the presence of disorder and its expansion is followed over time by fluorescence imaging. After a few years of experimental development, the first observations of Anderson localization in 3D emerged in 2011 in Urbana Champaign (USA), jointly with the Charles Fabry laboratory (France), and more recently, in 2015, at LENS in Florence (Italy).

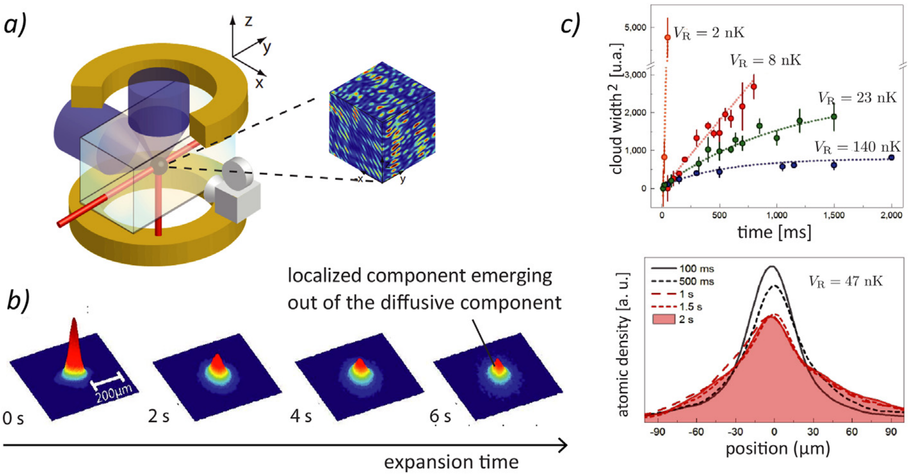


FIG. 5.8 – (a) Observation of Anderson localization in 3D at Charles Fabry laboratory, from F. Jendrejewski *et al.*, *Nat. Phys.* **8**, 392 (2012). The represented experimental setup includes a magnetic levitation (yellow coils) and two laser speckle fields (in blue) to achieve the most isotropic disorder possible (see the three-dimensional representation of the disordered potential). (b) Atomic density profiles showing the expansion of the atomic cloud at different times. The density profile is the superposition of two components: a diffusive part which spreads slowly, revealing in the center a localized part which remains frozen. This effect is due to the broadened energy distribution that extends across the mobility edge, as illustrated in figure 5.7b. (c) Similar observation at LENS, in Florence (Italy), from Semeghini *et al.*, *Nat. Phys.* **11**, 554 (2015). Top: square of the width of the cloud as a function of time ($\Delta r^2(t)$), for different amplitudes V_R of disorder. At sufficiently strong disorder the size saturates at long times, which is a signature of the localization. Bottom: density profile at different times, for a given disorder amplitude.

If these observations represent an undeniable first success for the study of the Anderson transition, they are, however, only a first step. Indeed, cold atoms have not escaped the experimental difficulties encountered in other systems, even if they are here of a different nature. The ideal situation would have been to show a clear transition between diffusive and localized behaviors by increasing the intensity of the disorder. But what is observed is different! If diffusion is well visible at weak disorder, the situation becomes more complicated at high disorder, when one approaches the Ioffe-Regel criterion. Indeed, in spite of the precautions taken, the switch on of an intense disorder induces a significant broadening of the energy distribution of the atoms around the mobility edge (green curve in figure 5.7b). This leads to the coexistence of a diffusive component and a localized component within the atomic cloud. In principle, it is therefore sufficient to wait for the diffusive atoms to spread away to reveal the localized part that remains frozen in the center (see figure 5.8b and c). The situation, unfortunately, turned out to be not that simple. Indeed, the diffusion coefficient D is typically very low for atoms whose energy is just above the mobility threshold (remember that D cancels precisely at the transition), and it is therefore necessary to wait for very long times to observe the localized component. In practice, up to 6 seconds were necessary in the experiments carried out at the Charles Fabry laboratory: an eternity for the typical time scales of ultra-cold atoms!

The broadening of the energy distribution in the presence of strong disorder has therefore been identified as a bottleneck in the study of the Anderson transition. On the one hand, having enough time to differentiate between the diffusive and localized components makes the experiments very difficult to perform. On the other hand, the energy broadening prevents the observation of the transport properties at a well defined energy, so that it is impossible to observe finely the critical regime around the transition. At first sight, goodbye to the measurement of the critical exponent! However, the situation is not fixed and new strategies are currently being considered to circumvent the problem. One of them, which uses a spectroscopic method to precisely populate the atoms at a given energy in the disorder, is under development at the Charles Fabry laboratory. It is also possible to change the paradigm and explore other ways, such as studying the localization properties not in the space of positions but in the space of velocities. This new route is the subject of the following section.

5.4 Coherent Backscattering: Visualizing Interferences

5.4.1 Localization in the Space of Velocities

In all experiments discussed above, the localization effects of the atoms in the disordered potential are observed in position space: an atomic wave packet is let spread and, at a sufficiently long time, its spatial density profile, exponentially localized by interferences, is visualized by fluorescence imaging.

A difficulty of this approach is, however, that it may be difficult to distinguish a manifestation of localization from a diffusive motion that would be, for example, very slow. In this context, as early as 2012 the idea was put forward that the microscopic interference mechanisms responsible for localization effects could be visualized *directly*, by probing the distribution of atomic velocities rather the atom positions. Following this idea, the experiment that is reciprocal to the one starting from a spatially narrow wave packet involves a cloud of atoms with a very narrow velocity distribution of non-zero mean value, so as to mimic a “plane-wave” type state. In practice, this configuration is achieved by cooling the cloud very strongly (a temperature as low as 150 nanokelvins was for example reached in the experiment shown in figure 5.9), and by accelerating it for a short time so to transfer him a finite mean velocity.

By virtue of the Heisenberg uncertainty principle, the resulting state is very extended spatially, so that no dynamics is observed in position space (the density profile remains always uniform on average). What about the dynamics of the velocity distribution? Scattering of the atoms on the potential being elastic, the absolute value of the mean velocity of the cloud remains constant, but its direction changes at each collision of an atom on the disorder (this is the manifestation of the random walk in the space of velocities). Within a classical picture, one therefore expects the directions of atomic velocities to be equiprobable, the velocity distribution taking the form of a two-dimensional ring, or a sphere in 3D. Like for the propagation in position space, however, this classical description is likely to be strongly modified by interferences between the different trajectories. The question is to know how! Since 2012, several theoretical and experimental works have explored this problem, which has proven to be very rich. In particular, the manifestations of localization in reciprocal space turn out to be different from – and just as spectacular as – their counterpart in position space.

5.4.2 Coherent Backscattering of Cold Atoms

Based on theoretical works developed by a French team at the CQT (Centre For Quantum Technologies) in Singapore, the evolution of an atomic cloud in velocity space was measured experimentally in 2012 by two French research teams, one at Institut de Physique de Nice and the other at Laboratoire Charles Fabry in Palaiseau. These experiments consisted in strongly cooling a cloud of dilute rubidium atoms to the condensed state, then applying a magnetic field gradient to the cloud so as to transfer it a non-zero mean velocity. The velocity distribution of the cloud in the presence of a laser speckle was then probed at different times with the time-of-flight imaging method. The results of Palaiseau experiment are presented in figure 5.9a. The initial velocity distribution, first of all, reflects the state in which the gas has been prepared: it is a narrow peak centered around mean velocity vector $\mathbf{v}_i$ of the cloud. This distribution evolves rapidly as soon as the optical speckle is switched on. One then observes a decrease of the initial peak and the appearance of a ring. This phenomenon, discussed above, signals the random walk of the atoms in the optical disorder (figure 5.1b): the atoms progressively lose the memory of their initial velocity, and after a few scattering events all velocity directions become equiprobable, with the constraint of keeping the absolute value of the velocity constant due to the elastic nature of the scattering process. As we have seen in the previous sections, however, the classical random-walk picture does not take into account atomic interferences. In figure 5.9a, a spectacular manifestation of these interferences is clearly visible in the last three velocity distributions: in the vicinity of the backscattering direction, one observes the emergence of a peak which, at sufficiently long times (a few milliseconds in practice), emerges clearly from the scattering ring. This phenomenon, called coherent backscattering, is caused by the interference between two paths involving the same multiple scattering sequence but traveled in opposite directions, as illustrated in figure 5.9b. This interference is perfectly constructive only for velocities $\mathbf{v}$ close to $-\mathbf{v}_i$. Indeed, when this condition is not fulfilled the two multiple scattering paths accumulate a slightly different phase, which makes the interference cancel on average.

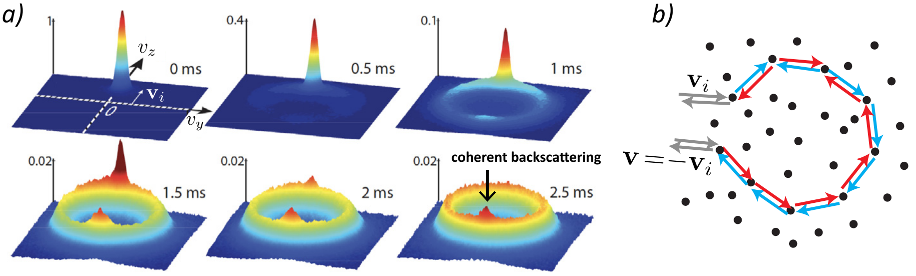


FIG. 5.9 – (a) Experimental velocity distribution of a cloud of ultra-cold rubidium atoms whose global velocity $\mathbf{v}_i$ is non-zero, measured at different times in the presence of a two-dimensional speckle light field. Because of elastic multiple scattering, the distribution becomes quickly isotropic. After a few milliseconds, one also observes the appearance of a coherent backscattering peak around the $-\mathbf{v}_i$ velocity direction. (b) Interference between counter-propagating multiple scattering paths responsible for coherent backscattering. From Jendrzejewski *et al.*, *Phys. Rev. Lett.* **109**, 195302, 2012.

The phenomenon of coherent backscattering is obviously not specific to cold atoms. It has been observed since the late 1980s in optics, in several experiments involving the propagation of light in suspensions or semiconductor powders. Later, coherent backscattering of acoustic and elastic waves was also detected. For classical waves, the experimental procedure usually consists in illuminating a disordered sample with a collimated beam and measuring the signal reflected from this sample in the far field. Nevertheless, cold atom experiments have at least two major advantages. First, no interface between the disordered medium and the outside is involved, the phenomenon being probed directly "inside" the disordered medium (*i.e.* in the optical speckle). The description of coherent backscattering thus does not require to take into account finite size effects which, in general, seriously complicate the interpretation of the results.

Another advantage of the method used for measuring coherent backscattering of cold atoms lies in the possibility to perturb, in a controlled way, the interference sequence of figure 5.9b, for example, by subjecting the cloud to a short pulse from outside. This idea has been put into practice in recent experiments at the Laboratoires Charles Fabry in Palaiseau and PhLAM (Laboratoire de Physique des Lasers, Atomes et Molécules) in Lille to make the coherent backscattering peak of a cloud of atoms disappear and reappear at well chosen times. Figure 5.10a shows, for example, how the coherent backscattering peak behaves when a magnetic field gradient is applied to the cloud for a short time. Upon switching on the magnetic field, the phase of the atoms is suddenly changed so that the interference is destroyed and the peak disappears. A little later, however, one observes a resurgence of the peak at the precise moment when the counter-propagating scattering paths re-synchronize. In a near future, this way of "probing" multiple scattering sequences could allow for direct control and visualization of the microscopic interference mechanisms at work in the physics of wave localization in disorder.

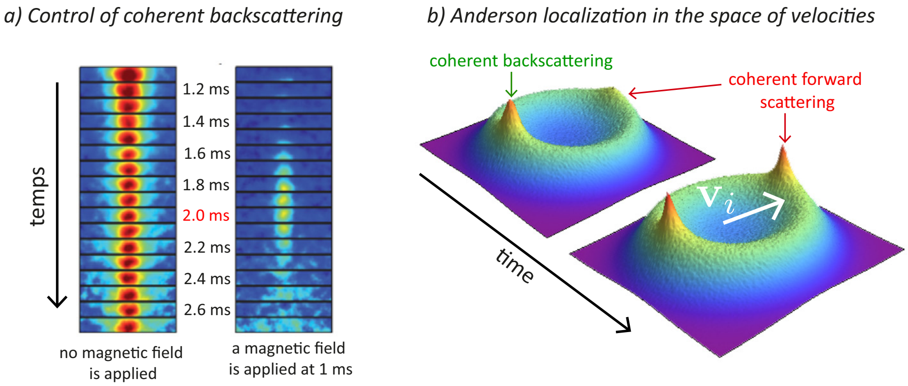


FIG. 5.10 – (a) Experimental images of the coherent backscattering peak of a cloud of ultra-cold atoms at different times, with and without a magnetic field gradient applied at time $t = 1$ millisecond. Without applied field, the peak does not evolve. When a field is applied, the peak first disappears, then reappears briefly a little later, when the phases of the interfering paths re-synchronize. Adapted from Müller *et al.*, *Phys. Rev. Lett.* **114**, 205301, 2015. (b) Theoretical velocity distributions obtained after propagation of a cloud of atoms in a two-dimensional speckle potential, at two successive times subsequent to the appearance of the coherent backscattering peak. In addition to the latter, a new peak grows around the forward direction $\mathbf{v} = \mathbf{v}_i$. This peak, visible only in the Anderson localization regime, is called the forward coherent scattering effect. Adapted from Ghosh *et al.*, *Phys. Rev. A* **90**, 063602, 2014.

5.4.3 Anderson Localization in the Space of Velocities

We have just seen that the observation of the velocity distribution of a matter wave provides a complementary and very visual picture of atomic multiple scattering in a disordered potential. It is also the natural framework to observe coherent backscattering. What about Anderson localization? We have explained above that, in position space, Anderson localization "freezes" the spreading of a wave packet. But what do we expect in the space of velocities? The answer to this question, which was explored theoretically in 2012, is surprising and unexpected. In the Anderson localization regime, the film in figure 5.9a keeps evolving and, at long time, when the atomic gas starts to experience Anderson localization, a *second* peak grows in the velocity distribution. The emergence of this extra peak is illustrated in figure 5.10b, which shows the theoretical velocity distribution expected at two successive times, subsequent to the emergence of the coherent backscattering peak. The additional peak appears around the forward scattering direction, *i.e.* around $\mathbf{v} = +\mathbf{v}_i$, hence the name "forward coherent scattering peak". The description of this phenomenon is much more complicated than for coherent backscattering. It can be interpreted as a kind of double coherent backscattering effect, in which the atoms of the backscattering peak are backscattered again, the process repeating itself many times. When the atoms propagate according to classical diffusion, this phenomenon is very unlikely and the peak is hardly visible. In the Anderson localization regime, on the other hand, the proliferation of interferences in multiple scattering brings the probability of this mechanism to 100%, and the peak becomes visible.

So far, no direct observation of the coherent forward scattering peak has been reported yet. Nevertheless, we mention that recently, a similar effect has been measured at the PhLAM laboratory in Lille, in an experiment involving atoms subjected to a pulsed standing wave (see section 5.5.3).

5.5 Cold Atoms and Disorder: Other Configurations

5.5.1 Universality of Localization Phenomena

Today, it is well established that Anderson localization is caused by the proliferation of interferences in a multiple scattering process. With this point of view, the localization of a matter wave in a disordered optical potential appears as a particular scenario. In fact, it is in principle possible to observe localization phenomena for any wave subject to a form of disorder. In the previous sections, we have already mentioned the case of electrons in solids with defects, as well as that of classical waves such as acoustic signals propagating in elastic lattices. In order to stay within the framework of atomic physics, we will now focus on two other interesting configurations involving the use of cold atoms in the search for wave localization.

5.5.2 Light Scattering by Cold Atoms

In optics, several groups suggested in the late 1990s that atomic clouds themselves should be excellent candidates to realize a disordered medium for light. This scenario is, in some way, the reverse of the one we have considered so far: atoms now play the role of the disordered medium, and light the role of the scattering wave. The multiple scattering process consists in this case in a succession of spontaneous absorption/emission cycles of the light on the atoms. One of the main motivations for using atoms to scatter light is that they constitute almost ideal scatterers: they are point-like and can be excited around a well-defined transition (see chapter 3). For light resonating with such a transition, the atomic cross section becomes very large, of the order of the square of the optical wavelength. This allows to obtain the large optical thicknesses required to reach the multiple scattering regime.

Unlike the problem of multiple scattering of atoms in an optical disorder, probing scattering of light directly inside a disorder made of atoms is complicated. For this reason, experiments in this field in general impose to detect the wave at the exit of the medium. Precisely, one measures the luminous flux transmitted or reflected by a cloud of atoms illuminated by a laser beam, see the illustration in figure 5.11a. As for matter waves, in the low disorder regime where $kl^* \gg 1$, the light intensity obeys a classical diffusion equation with diffusion coefficient D (k is now the wave number of the incident beam and l^* the mean free path of the light propagating through the atomic cloud). A common strategy to characterize this process is to cut off the incident laser at a certain time and then record the time decay of the signal transmitted by the cloud. For a classical diffusion process this decay is exponential, controlled by the diffusive mode of longest lifetime, which is of the order of R^2/D where R is the typical size of the cloud. An experimental observation of this phenomenon at Institut Non Linéaire de Nice is shown in figure 5.11a.

Multiple scattering on atoms has also been studied in the context of coherent backscattering of light. The latter was observed for the first time in a cloud of rubidium atoms in 1999 at Institut Non Linéaire de Nice. The interference signal measured in this experiment is reproduced in figure 5.11b. For this measurement, the atoms have been cooled to temperatures in the millikelvin range (the gas is thus cold, but not as cold as in the experiments discussed in sections 5.3 and 5.4). This cooling is imposed by the fact that, at too high a temperature, the atomic scatterers move. This imprints a phase shift to the optical wave, which tends to destroy the interference between reversed paths. In practice, maintaining a constructive interference requires that the typical distance traveled by the atoms during a light scattering process is much smaller than the optical wavelength. Notice, in passing, that cooling the atoms is also necessary to observe the classical diffusion of figure 5.11a. Indeed, at high temperatures a redistribution of the scattered frequencies takes place because of the Doppler effect. Therefore, the propagation in the disorder is no longer characterized by a unique mean free path but rather by a distribution of mean free paths, which changes the very nature of diffusion. Coming back to the coherent backscattering effect of figure 5.11b, it is interesting to note that the peak contrast is much lower than the one obtained with atomic matter waves (figure 5.9). This is due to the internal quantum structure of the atomic scatterers combined with the polarization degree of freedom of the optical wave: for some photon multiple scattering trajectories on a given atomic sequence, it can happen that the probability amplitude of the reversed path is different because of the selection rules of atomic transitions. The net effect of this imbalance in the amplitudes of reversed paths is a reduction of the contrast of the backscattering peak.

Beyond coherent backscattering, the question that naturally comes to mind is that of Anderson localization of light in a cloud of atoms. The problem is all the more relevant since many experiments of photon localization in disordered media made of classical scatterers (often powders of semiconductor materials) have been questioned, as the effects observed in these media can be explained by the presence of absorption or fluorescence. In this context, ensembles of atomic scatterers seem to constitute an especially simple and promising type of disorder to explore Anderson localization of light. Recent numerical studies, however, have revealed a surprising result: in three-dimensional disordered media consisting of point scatterers like atoms, dipole–dipole interactions prevent Anderson localization from occurring! On the other hand, a slight decrease in these interactions (obtained, for example, by applying a magnetic field lifting the degeneracy between excited Zeeman sublevels of an atomic transition) allows to restore the phenomenon (provided, again, that the temperature of the atoms is low enough). These recent predictions show the great richness of the problem of the interaction between light and dense atomic ensembles, which constitutes today a very open field of research.

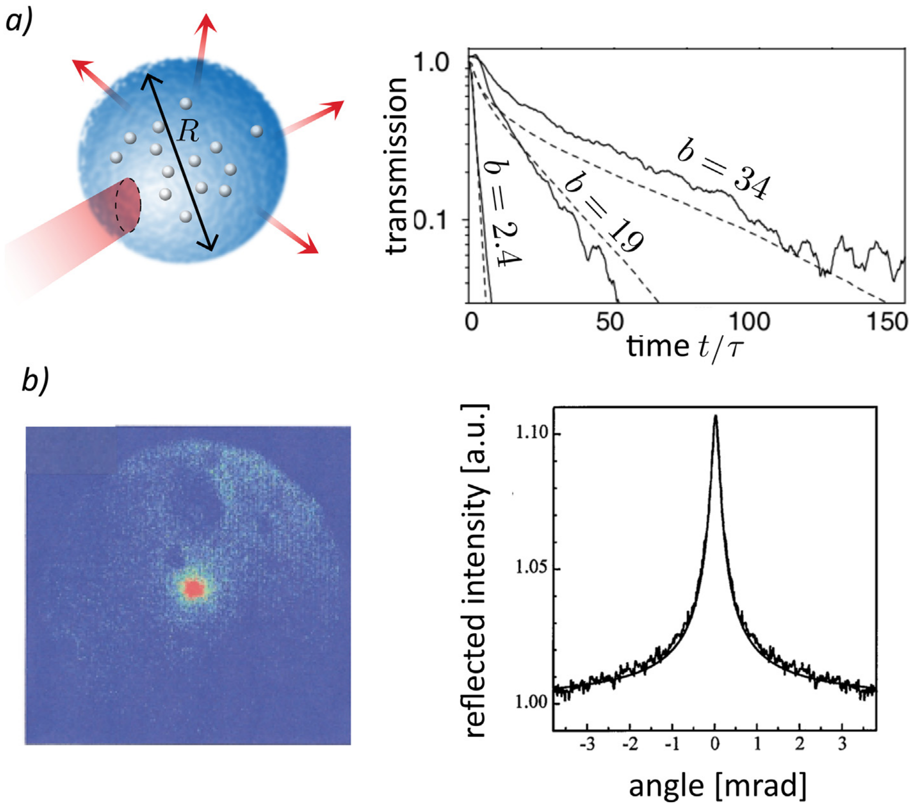


FIG. 5.11 – (a) Experiment of classical light scattering on a cloud of atoms (from: Labeyrie *et al.*, *Phys. Rev. Lett.* **91**, 223904, 2003). A laser beam illuminating the cloud is cut off at some initial time. In the classical diffusion regime, this leads to an exponential decay of the transmitted optical signal in time, with a characteristic rate of the order of R^2/D, where R is the typical size of the cloud and D the diffusion coefficient (in the figure, time is expressed in units of $\tau = l^*/c$, the average time interval between two collision processes of the wave on the atoms). The R^2 dependence of this rate is verified by varying the optical thickness $b = R/l^*$ of the cloud. (b) By illuminating the atomic cloud with a collimated beam, a coherent backscattering peak is observed in the angular distribution of reflected intensity. Image (left) and profile (right) of the optical coherent backscattering peak (from Labeyrie *et al.*, *Phys. Rev. Lett.* **83**, 5266, 1999).

5.5.3 "Kicking" Atoms to Localize Them

Another way of exploiting cold atoms in the search for localization phenomena was put into practice in the mid-1990s, based on theoretical works developed in the late 1970s in the context of quantum chaos. The idea is to replace the spatial disorder by a form of *temporal* disorder consisting in subjecting a cloud of atoms to a pulsed standing wave, which transmits to the atoms recoil pulses or "kicks". This system is called the "atomic kicked rotor" because, in the classical limit, the equations of motion are identical to that of a pendulum to which one would periodically transmit short pulses. Within a classical description, the kicked rotor displays a chaotic dynamics when the kicks are strong enough. Indeed, in this limit, a kicked atom moves over a large distance and thus ends up at a completely different position in the standing wave, which strongly modifies the amplitude and the sign of the next kick. Over a sufficiently long time, the atom is thus subjected to a series of kicks of quasi-random amplitudes. This induces a quasi-random walk of its momentum and thus a diffusion process. Chaos thus plays the role of disorder in this system. Let us note that, strictly speaking, the atomic kicked rotor is a perfectly deterministic system. Nevertheless, the fact that it involves a set of atoms with different initial conditions and chaos makes, in practice, the evolution of the atomic momentum indistinguishable from a true random walk.

The richness of the kicked rotor can be seen in its quantum dynamics. Indeed, while in the classical limit the evolution of momenta is diffusive in nature due to chaos – in other words, the momentum dispersion Δp^2 increases linearly with time, in a way analogous to equation (5.1) –, for the quantum evolution the momentum dispersion saturates at long times, Δp^2 reaching a constant value. This phenomenon, dubbed dynamical localization, is completely similar to Anderson localization, except that it occurs in momentum space and not in position space. Its origin is also the same: it is due to the proliferation of interference between chaotic multiple scattering trajectories.

In its standard version, the atomic kicked rotor is a one-dimensional system (along the axis of the standing wave), so that it displays one-dimensional Anderson localization. The latter was first observed experimentally with kicked atoms in the mid-1990s, in Mark Raizen's group in Austin, USA, before the advent of ultra-cold atoms. This experiment, in particular, well demonstrated the exponential localization of the distribution of atomic momenta under the effect of the kicks, as illustrated in figure 5.12.

In parallel to these seminal measurements, the question soon arose whether the atomic kicked rotor could be modified in a simple way to obtain an analogue of the Anderson phase transition expected in three-dimensional disordered systems. A positive answer to this question was given by theorists in the late 1980s. The idea was to replace the three-dimensional disorder by a sequence of kicks in three *temporal* dimensions, which is much simpler to realize experimentally. The corresponding model is a kicked rotor in which the strength of the kicks is modulated by a quasi-periodic function of time. A typical sequence of kicks to which the atomic cloud is subjected in this "quasi-periodic" kicked rotor is illustrated in figure 5.13a. In this system, an Anderson phase transition is present. It separates a regime where the atoms follow a chaotic diffusion in momentum space, from a localization regime where the momentum distribution is frozen. Note that unlike atoms evolving in a disordered potential, the parameter allowing to switch from one regime to the other

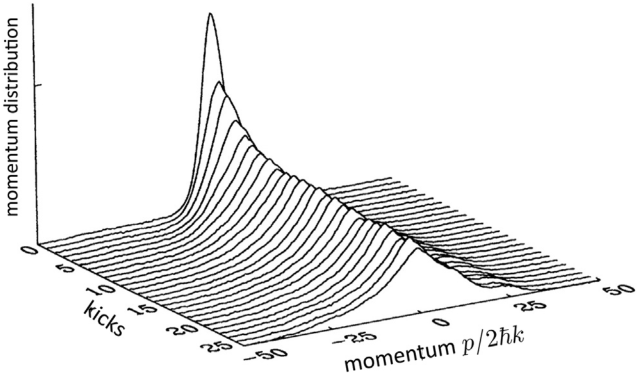


Fig. 5.12 – First experimental observation of one-dimensional Anderson localization of sodium atoms in the atomic kicked rotor. After a certain evolution time, *i.e.*, a certain number of kicks, the atomic momentum distribution freezes and becomes exponentially localized. Here momenta are measured in units of the recoil momentum of the atom. Adapted from Moore *et al.*, *Phys. Rev. Lett.* **75**, 4598 (1995).

is no longer the product kl^* – see equation (5.6) – but the kick strength. This implies, in particular, that it is not required to reach temperatures as low as for atoms in disordered potentials (in particular, for atoms of bosonic statistics it is not necessary to reach the condensation threshold).

The experimental realization of a quasi-periodic kicked rotor with cold atoms was carried out at the end of the 2000s at the PhLAM laboratory in Lille. This work constitutes the first detailed experimental study of the Anderson transition. In a first series of measurements, the researchers were able to follow the evolution of the momentum dispersion of a cloud of cesium atoms in the diffusion and localization regimes, as well as the evolution at the critical point of the Anderson transition where the temporal behavior is intermediate, see figure 5.13b. On this question, we have seen in section 5.3 that for atoms in a spatial disordered potential the energy dispersion of the cloud makes the characterization of the Anderson transition difficult. In the kicked rotor this problem does not arise, because the transition from one regime to the other is achieved by changing the kick strength, which does not depend on energy.

Further studies by the team in Lille have also allowed for measurements of the critical exponent of the Anderson transition, the result of which is in good agreement with numerical predictions. The universality of the value of this exponent has also been demonstrated experimentally. Finally, it should be mentioned that in very recent works, the atomic kicked rotor has been exploited to measure an analogue of the coherent backscattering and the coherent forward scattering peaks of cold atoms. By an ingenious temporal modulation of the kick sequences applied to the atoms, it has also been shown that kicked atoms could be used to produce artificial gauge fields, and study their impact on Anderson localization.

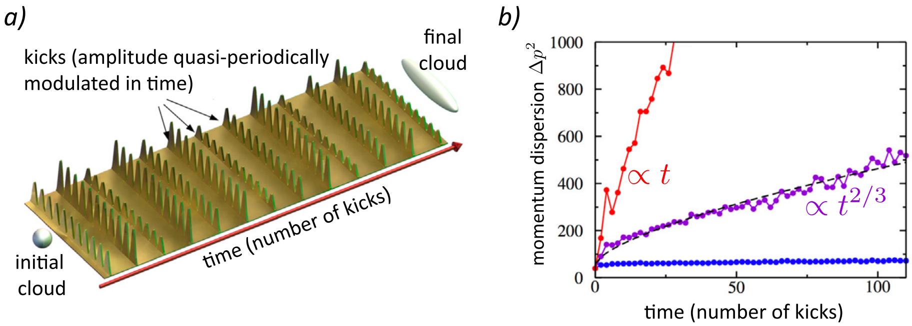


Fig. 5.13 – Experiment of kicked atoms aiming to probe the three-dimensional Anderson transition. (a) Principle: a cloud of atoms is subjected to a periodically pulsed standing wave, whose amplitude is modulated quasi-periodically in time. The system displays the analogue of an Anderson transition, which is detected by varying the strength of the kicks. (b) Momentum dispersion of the kicked atomic cloud as a function of time, in the classical diffusion regime (red dots) where $\Delta p^2 \propto t$ – see equation (5.1) – and in the localization regime (blue dots) where Δp^2 saturates at long times. At the critical point of the Anderson transition (purple dots), the evolution is intermediate, $\Delta p^2 \propto t^{2/3}$. From Chabé *et al.*, *Phys. Rev. Lett.* **101**, 255702, 2008.

5.6 Interactions and Disorder: When Atoms Talk to Each Other

The behavior of atomic gases under the combined effect of disorder and interactions is a rich and multifaceted problem, for which researchers still have only a partial picture. The great potential of cold atoms to explore this question was identified early on, since in addition to the possibility of realizing optical disordered potentials, the technique of Feshbach resonances (see chapter 4) also provides a control of interactions for certain species of atoms. On the coexistence of disorder and interactions, different questions can be asked. A first one concerns the nature of the ground state of an interacting, ultra-cold gas in a disordered environment. Since the first theoretical works of the end of the 1980s, this problem has sparked much interest, with many experimental results obtained recently. Beyond the case of the ground state, in the last decade physicists have also been interested in the excited states of interacting disordered gases, with the major theoretical discovery in 2006 of the existence of a non zero temperature phase transition for conduction electrons in metals. This phenomenon is now known as many-body localization. In this last section, we briefly discuss these problems, which are still largely open.

5.6.1 Quantum Phases of Disordered Gases at Low Temperatures

In 1989, theorists wondered how should a zero-temperature Bose gas behave in the presence of interactions and disorder. In this framework, one of the simplest systems is a one-dimensional gas in an optical lattice. Atoms can tunnel from a site to another, and the weight of interactions is controlled by modulating the amplitude of the lattice. Disorder, finally, can be added simply by making the lattice potential quasi-periodic, as discussed in section 5.2.1. The physics of this system in the absence of disorder is now well understood. It has been described in chapter 4, and we recall it quickly here. For weak interactions, the ground state of the gas is superfluid: the atoms can easily move from one site of the lattice to the other, they are completely delocalized on the lattice. The number of atoms on each site is thus very fluctuating, which, according to the Heisenberg uncertainty principle, imposes weak phase fluctuations. This state is relatively robust against interactions: to break it, the interactions must be increased to a threshold beyond which the gas becomes strongly correlated. At this threshold, a phase transition known as the Mott transition appears: because of the strong interactions it becomes energetically prohibitive for the atoms to move from one site to another. They remain stuck on a given site, unable to move due to repulsive interactions with their neighbors. When this happens, the superfluidity is destroyed and the gas becomes an insulator.

To understand how this scenario is modified in the presence of disorder, it is useful to come back to the physics of a disordered Bose gas that we have discussed in the previous sections. At zero temperature, the one-dimensional gas is an Anderson insulator, its quantum states are exponentially localized in space. At very weak interactions, the gas of bosons condenses in the localized states of lowest energy, forming well separated islands of superfluid. The system thus formed is not really an Anderson insulator anymore, since it presents, locally, well coherent superfluid regions. On the other hand, it is not completely a superfluid either, since the separation of islands prevents the appearance of a long range coherence. This peculiar state of matter, intermediate between a superfluid and an insulator, is called a Bose glass. The transition to the physics of the superfluid or of the Mott insulator is then the following. When interactions are increased more and more, the islands of the disordered gas eventually touch each other and the coherence of the fluid is restored: one recovers a superfluid behavior. When the disorder is very large, however, the interaction energy necessary for the islands to touch each other becomes so strong that atoms get stuck again on their sites: the Bose glass then looks more and more like a Mott insulator, and the superfluid regime is never reached.

The phase diagram of interacting Bose gases in a one-dimensional disordered lattice summarizing these discussions is represented in figure 5.14a. It was established qualitatively at the end of the 1980s, and was subsequently confirmed and refined by several theoretical and numerical approaches. Note that the various transitions between the superfluid, Mott insulator or Bose glass phases have many interesting properties that we will not discuss here. On an experimental level, several teams have also explored this diagram. Figure 5.14b shows results obtained at LENS in Florence in 2014 by measuring the coherence of a potassium gas in a quasi-periodic lattice. These measurements qualitatively reproduce the theoretical phase diagram. Note, however, that in this experiment the gas is trapped in a harmonic potential which transforms the true phase transitions into soft transitions or “crossovers”. On the other hand, the number of atoms per lattice site is not fixed

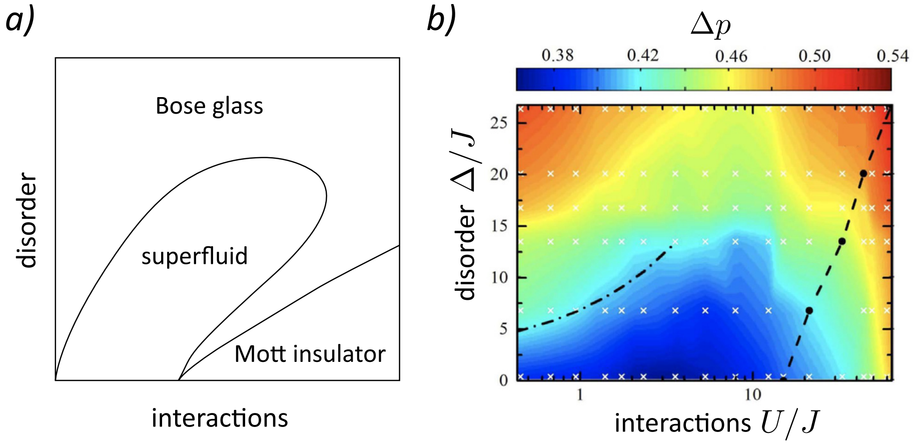


FIG. 5.14 – (a) Schematic phase diagram expected for a gas of interacting bosons at equilibrium in a disordered optical lattice in 1D (adapted from Cazalilla *et al.*, *Rev. Mod. Phys.* **83**, 1405, 2011). (b) Experimental measurements of the width Δp of the momentum distribution of a potassium gas in 1D, in the presence of a quasi-periodic lattice. Δp is plotted as a function of the amplitude U of interactions and the amplitude Δ of disorder. These amplitudes are expressed in units of probability J of moving from one site to another in the lattice, and Δp in units of the inverse of the lattice step. The width Δp is a measure of the coherence of the gas. The measurements highlight the coherent superfluid phase in blue. The dotted lines are numerical predictions indicating the expected transitions to the Bose glass phase and to the Mott insulator phase (the latter is not visible due to experimental conditions). Adapted from D'Errico *et al.*, *Phys. Rev. Lett.* **113**, 095301, 2014.

in the experiment, which makes it difficult to observe the Mott insulator phase (which exists only for an integer number of atoms per site).

5.6.2 Many-Body Localization: When Disorder Makes Thermal Equilibrium Impossible

In the last decade, an important theoretical activity has emerged around the dynamics and the non-zero temperature behavior of interacting disordered quantum gases. This activity has been motivated by the major discovery, in 2006, that the energy spectrum of an interacting disordered system could present a transition between a conducting phase and an insulating phase in dimension one, a bit like the Anderson transition of non-interacting disordered systems in dimension three (see section 5.3.4). The insulating phase in question is called "many-body localization" (MBL) phase. Unlike the phase transitions discussed in the previous section, the transition between the conducting phase and the MBL phase does not concern the ground state but appears at non-zero energy in the spectrum. The existence of this transition has been demonstrated by a large amount of numerical works using lattice disorder models. Figure 5.15a reports very complete numerical results obtained in a chain of interacting spins subjected to a random magnetic field playing the role of disorder. The spectrum of this system shows a phase transition between a conducting phase (called "ergodic" in the figure) and the MBL phase. Even if the properties of the MBL transition are still largely unknown, some results seem to be established today. First, like in disordered systems without interaction, in the MBL phase transport is frozen at sufficiently long times. This property, observed for the first time with a one-dimensional gas by Immanuel Bloch's team in Germany, has also been measured recently in a gas subjected to a two-dimensional disordered optical potential. This last experiment is illustrated in figure 5.15b: a cloud of atoms, prepared in the form of a half-disk, is let to evolve under the effect of interactions in the presence or in the absence of disorder. In the absence of disorder, the memory of the initial state is quickly lost. In the presence of disorder on the contrary, the spread of the half-disk freezes.

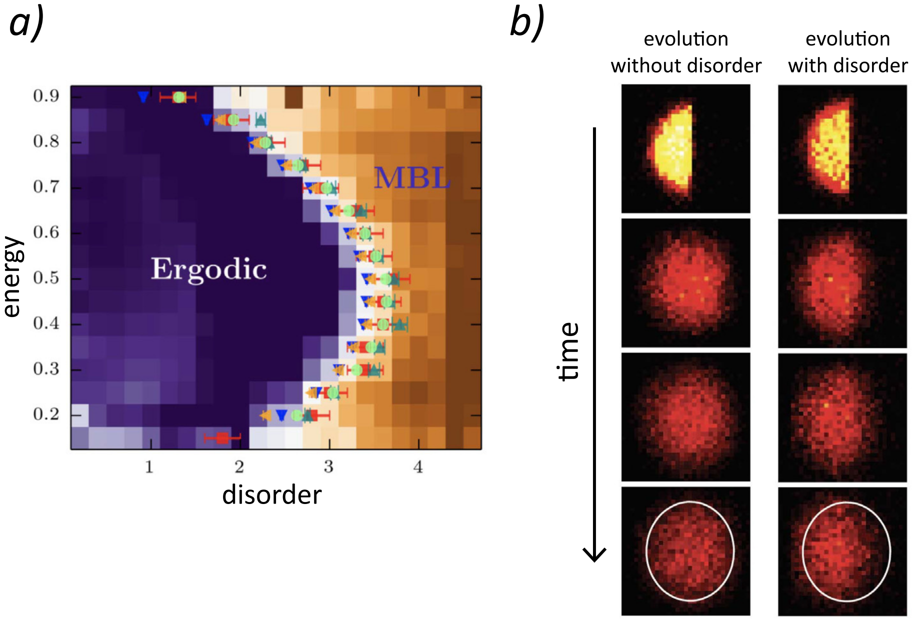


FIG. 5.15 – (a) Energy spectrum of an interacting spin chain subjected to a random magnetic field playing the role of disorder (from Luitz *et al.*, *Phys. Rev. B* **91**, 081103, 2015). Depending on the disorder amplitude, the states of the system can be localized ("MBL" phase) or delocalized ("ergodic" phase). The symbols, obtained by a numerical scaling analysis applied to different observables, indicate the position of the transition between the two phases. (b) Experimental density profile of an interacting two-dimensional ultracold atomic cloud, initially prepared as a half-disk (top images). In the absence of disorder (left profiles), the atoms thermalize due to interactions, which rapidly induces a uniform spatial distribution, independent of the initial state. On the contrary, in the presence of disorder (right profiles), the gas does not thermalize and keeps a memory of the initial state, signature of many-body localization (adapted from Choi *et al.*, *Science* **352**, 1547, 2016).

Many-body localization is nowadays a major research topic, going beyond the simple framework of the physics of disordered systems. It raises, in particular, crucial fundamental questions related to the dynamics of isolated, many-body quantum systems. For example, statistical physics teaches us that most isolated quantum systems naturally thermalize under the effect of interactions, in the sense that any sub-part of the system acquires an equilibrium temperature due to its interaction with the rest of the system. This is the "eigenstate thermalization principle", verified in particular in the conducting phase of the MBL transition. This principle is, however, violated in the MBL phase. Because of Anderson localization, the system cannot really thermalize and the final equilibrium state in general retains some memory of the initial conditions.

5.7 Conclusion

The natural complexity of disordered systems is a breeding ground for a very rich variety of physical phenomena, as briefly discussed in this chapter. This is true for systems of independent particles in the presence of disorder, and even more for systems of interacting particles, for which theoretical and experimental descriptions are still very patchy. In this respect, the use of cold atoms is extremely valuable, since it allows to study the physics of complex systems in the ideal scenario where the atoms are isolated from their environment and the disorder is well controlled *via* the use of various optical potentials, which in other contexts is in general difficult. In particular, most recent cold atom experiments are very close to being true quantum simulators. They should soon be able to systematically explore the many-body problem in the presence of disorder, known to be one of the most difficult of condensed-matter physics. In optics, we have seen that cold atomic clouds can also be used as ideal disordered ensembles for light. The story, in this context, is still very far from being finished since Anderson localization of light in dimension three, and the associated transition, has not yet been observed in ensembles of atoms, nor in any other system!

Chapter 6

Trapping and Cooling Ions

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Invented more than fifty years ago, ion traps are today the tools of choice for a large field of applications ranging from analytical instruments for pharmacology and biochemistry to the latest developments in physics research for computer and quantum simulations, high precision measurements and even the monitoring of chemical reactions at extremely low temperatures. Their success is built on the possibility to control all experimental parameters with precision, as well as on their great versatility allowing the storage of any charged particle from mesoscopic systems such as MEMS (microelectromechanical systems), dust, nanoparticles, as well as molecular and atomic ions, elementary particles such as protons or electrons and even antimatter. The ion trap has paved the way for many important developments and applications, with international recognition of the trap pioneers. The reader can find introductions to the subject on the website of the Nobel Foundation, with the 1989 prize awarded to Wolfgang Paul and Hans G. Dehmelt and the one awarded to David J. Wineland and Serge Haroche in 2012. In addition to these outstanding distinctions many essential contributions have been made by other physicists among whom we can mention Peter Toschek, the first to observe a single ion, Herbert Walther, pioneer of the crystallization of individual ions, or Günter Werth, a pioneer of precision atomic spectroscopy for decades (see figure 6.1).

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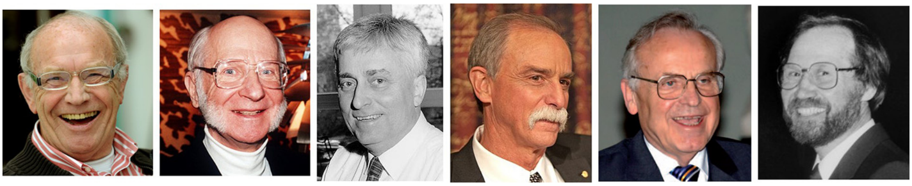

FIG. 6.1 – From left to right: Wolfgang Paul, Hans Dehmelt, Peter Toschek, Dave Wineland, Herbert Walther, Günter Werth.

In this chapter, we describe how to create, trap, illuminate, observe, cool, manipulate, and finally interrogate an ion in a trap, with a particular focus on electrodynamic traps.

Let us first look at how to create ions. The positive charge of the atomic nucleus and the negative charge of the surrounding electrons compensate each other, and an atom is therefore in general electrically neutral. It is possible, by collisions with other atoms, or interactions with a beam of electrons or light, to remove an electron from an outer layer of an atom or molecule. The total charge of the particle then becomes positive, a positive ion. Among many possible examples, we can cite the atomic ions Be^+, Ca^+, Sr^+, the molecular ions H_2^+, MgH^+, ... Note that it is possible to remove several electrons from an atom and to produce multi-charged ions like Ca^{2+} and even, in the most extreme cases, to remove all the electrons to keep only the naked nucleus as in the case of uranium U^{91+}. Some atoms or molecules agree to attach an extra electron, which gives rise to negative ions such as negative hydrogen H^-, lanthanum La^-, but in general these negative ions do not live very long, mainly because of collisions that make them lose their extra electron quickly.

The ion being created, now let us trap it! An ion, like any charged particle, is sensitive to electric field $\vec{E}$ and to magnetic field $\vec{B}$ through the Lorentz force $q\left(\vec{E} + \vec{v} \wedge \vec{B}\right)$ where q is the charge of the ion and $\vec{v}$ its speed. This property is used either to accelerate and guide the ions in beams circulating for example in storage rings, or to enclose them in an electric or magnetic cage and keep them there for a very long time (*Ionenkäfig* – ion cage – was the German term introduced by W. Paul, inventor of the trap which bears his name). Nowadays the term "ion trap" is the most common designation.

Today ion traps come in two distinct versions, Penning traps which use static electric and magnetic fields and Paul (or radio frequency) traps which use static electric fields and electric fields oscillating very rapidly. Both versions can confine particles for hours and days or even a few months, and thus are great tools for studying ions, especially for precision measurements that require long observation times or a large number of interrogations. These traps can operate at ambient pressure and confine charged dust particles or lycopods (almost perfectly round spores for public demonstrations), and allow to levitate mesoscopic objects that can be studied without any material support; they can work at reduced pressure to confine flu virus or enzymes, or even with a very high vacuum (a few millionths of a billionth of an atmosphere) to store atomic ions or small or large molecular ions. Traps are also installed at CERN where they trap very rare isotopes, elementary particles, or antimatter.

For all these cases, the size of the sample is an issue: if you trap several particles of the same charge, they will repel each other because of the Coulomb force, and therefore they cannot constitute a sample as dense as a cloud of neutral atoms. In a large trap, we typically trap a million ions, but we can very easily vary this number and make smaller and smaller ion clouds and, either by creating as few ions as possible or by ejecting a few ions from a larger cloud, obtain an individual ion in the trap.

And once trapped, what do we do with these ions? In the second part of this chapter, we will show some exciting applications that populate the labs today and contribute to the ever-growing success of ion traps. But first let us get to the heart of the trap: how does it really work?

6.1 How to Confine a Charged Particle?

In this section we explain how ion traps work by considering the case of positive ions. It is straightforward to adapt the parameters, essentially the polarity of the static electric fields, to trap negative particles.

The two types of traps described here were developed in parallel in the 1950s by Wolfgang Paul and Hans G. Dehmelt. The original purpose of these two types of traps was to serve as mass filter to isolate atoms of given mass. This is indeed possible because the mechanical action of electric and magnetic fields depends only on the charge-to-mass ratio q/m of the ion considered. The development of Paul and Penning traps has been very successful, and these instruments have been rapidly adopted for various scientific and industrial applications, including mass spectrometry for analysis in chemistry, particle accelerator physics, precision measurements in atomic physics and most recently quantum information processing.

In their original version, both types of traps share the same electrode geometry. They are composed of a ring surrounded by two endcaps as can be seen on the left side of figure 6.3. All surfaces are hyperboloids. With this particular shape, applying a potential difference U between the ring and the two endcaps (which are electrically connected), results in an electrostatic potential given by the formula

$$V(x,y,z) = U\frac{x^2+y^2-2z^2+2z_0^2}{r_0^2+2z_0^2}$$

where r_0 is the inner radius of the ring and z_0 is the minimum distance between the two endcaps, the origin of the coordinates being located at the center of the trap.

6.1.1 Penning Trap

The Penning trap was named by Hans Dehmelt after F. M. Penning, a Dutch physicist who made a proposal for magnetic field trapping in 1936. In the Penning trap, a magnetic field is applied along the z axis of the trap. In this configuration a charged particle will make a circular motion around the field lines, described by cyclotron frequency f_c, which depends on magnetic field B and the charge to mass ratio q/m of the trapped particle according to the formula $f_c = qB/2\pi m$. It is then sufficient to apply a positive voltage to the endcaps **relative to the ring** to keep positive ions in the center of the device. If the magnetic field is strong enough (around 1 T), the ions have no possibility to escape from this magnetic cage and will continue to rotate around the magnetic field lines.

The main commercial application of the Penning trap is mass spectrometry for the analysis of chemical composition of samples. To do so, any sample composed of various species is ionized, and stored in a Penning trap where each ion species has its own cyclotron frequency. The image current induced in the trap electrodes is recorded and analysed by a Fourier transform. This will map the cyclotron frequencies composing the signal, and thus the q/m ratios of the species present in the sample. The ultimate refinements of this method are described in paragraph 6.4.1.

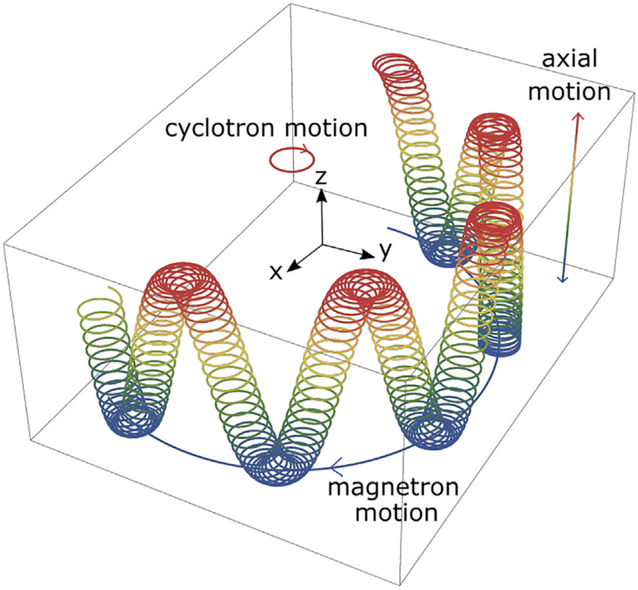

FIG. 6.2 – Ion trajectory in a Penning showing the axial motion along $0z$, the cyclotron and magnetron motions. The typical amplitudes of these motions scale from few micrometers to few millimeters.

6.1.2 Paul Trap or Radiofrequency Trap

The second type of trap is the radio frequency trap or Paul trap. It does not use a magnetic field, only electric fields, but in a very clever way as we will see. With a time-independent electric field like the one in figure 6.3, the effect of the electric force is to push the positive ions away from the ring (electrode (+)) and accelerate them towards the endcaps (electrode (−)). An equilibrium of charges in the center of the trap is then not possible. Wolfgang Paul's great idea was to use an alternating electric field that varies very rapidly in time. Let us imagine a positive ion close to the center of the trap at time $t = 0$ at a moment when the endcaps show a negative voltage and the ring a positive voltage. This ion will be attracted by the endcaps, but before reaching one of them, the polarity of the voltages will change sign, and the ion will be attracted by the ring and repelled by the endcaps. If the oscillation frequency of the electric field is well chosen, the net effect on the ion is

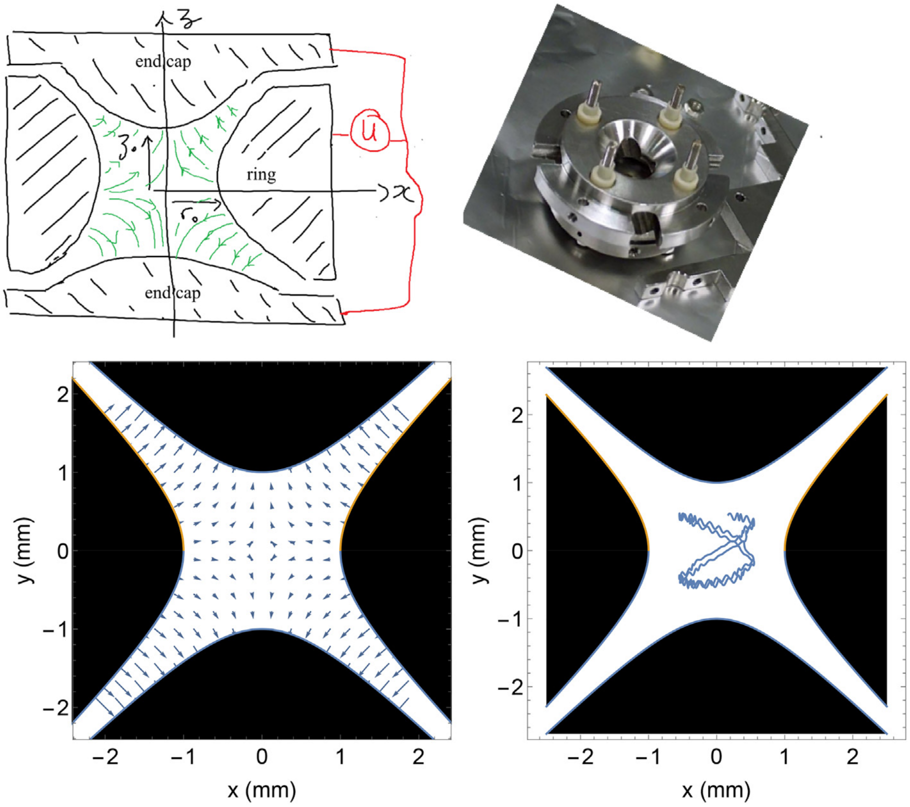

FIG. 6.3 – Top left: schematic view of a hyperbolic Paul trap. The electrical connections are in red. Top right: a practical realization where the inner diameter of the central ring is 8.4 mm. The white ceramics are used for the electrical insulation between the different electrodes of the trap. Bottom left: the black lines show the shape of the electrodes, the arrows indicate the direction of the electric field, thus the force experienced by a positive ion at a time t. Bottom right: trajectory of a trapped ion. The large amplitude motion is the macro-motion, the small oscillations are the micro-motion. We can see that the amplitude of the micro-movement is small at the center of the trap, and grows as the ion moves away from the center.

an average force that pulls it towards the center of the trap and prevents it from escaping: it is stored! The experimentalist must choose a confinement frequency adapted to the trapped particle, high frequencies (1–60 MHz) for light particles (atomic or molecular ions), intermediate frequencies (10 kHz–1 MHz) for mesoscopic particles and low frequencies (50–1000 Hz) for heavy particles (lycopod powder or dust particles).

The characteristic motion of an ion trapped in a Paul trap can be decomposed into a slow macro-motion caused by the effective trapping force of the trap and a faster micro-motion due to the fact that the ion is driven by the oscillating force created by the alternating electric field of the trap. The amplitude of the micro-motion grows with the amplitude of the electric field, and with the ion's distance from the trap center. For high-precision measurements, it is essential, to keep the object under study at rest and thus to eliminate the micro-motion, *i.e.* to place the ions at the null of the radio-frequency field. In a trap of hyperbolic geometry, the field cancels only at one point: the center of the trap. As a consequence, the ideal condition for immobilization can only be satisfied for a single ion, which is a limiting factor for the experiments. Moreover, hyperbolic traps have the disadvantage of being closed, solid structures, and holes have to be drilled in the electrodes to admit atoms or laser beams, which will perturb the trap operation.

It is possible to solve these structural problems by changing the geometry of the trap electrodes, choosing a linear Paul trap like the one shown in figure 6.4. In such a trap, the oscillating electric field has zero amplitude along the central axis of the trap. Ion chains can be confined in such a trap under ideal conditions, in particular to realize quantum bit registers for quantum information processing or to realize spectroscopic measurements without line broadening by the Doppler effect.

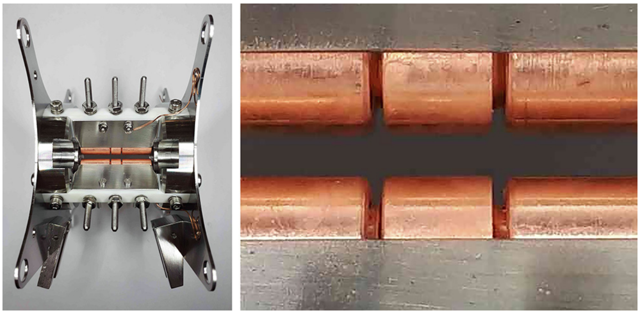

Fig. 6.4 – Left: Linear Paul trap developed for the GiantMol project at Aix-Marseille University. Right: zoom on the trapping electrodes. They are copper cylinders of 5 mm diameter. The right and left segments are equivalent to the endcaps, and the central segment is equivalent to the ring of the hyperbolic trap. The central segment is 4 mm long.

6.1.3 Trap Zoology

Beyond the hyperbolic or linear traps, there is a whole zoology of radiofrequency traps, whose geometries have been designed by the constraints of the targeted applications. Different examples of traps are shown in figure 6.5.

Miniature traps with reduced electrodes such as the endcap trap or ring trap (a) and (b) in figure 6.5 are solutions for creating extremely open structures that allow the introduction of many (laser) beams.

Microfabricated Surface traps – where the electrodes are realised on a printed circuit board – are an easily adaptable solution for applications related to quantum information manipulation. Indeed, these applications need traps as small as possible and with many trapping zones to be able to store and let interact as many ions as possible on the smallest possible surface (figure 6.5c). Very soon after the first demonstrations of ion-based quantum logic gates, efforts to increase the number of probed ions triggered the realization of very compact modular traps. Surface traps for which all electrodes are in the same plane can be realized by on-chip microfabrication techniques. The design and the custom fabrication of the traps allow to adapt the storage potential by the geometry of the electrodes. This solution is crucial for the realization of traps with many electrodes required to control quantum registers, and presents a very open structure to probe the ions by laser beams. The proximity of the ions to the trap surfaces in these micrometer-sized structures has revealed new physical effects that perturb the ions when they are confined near the electrode surface. The scientific community has taken up this issue in a joint effort to work on the quality of the surfaces to solve the problem and to use the extreme sensitivity of the internal quantum state of the ions to probe the properties of the surfaces.

Multipole traps For other applications, it may be interesting to have a very large trapping volume in which the ions are perturbed as little as possible by the trapping fields, in order, for example, to study the kinetics of chemical reactions. In this case, the multipole trap, a type of linear trap with more than 4 rods (typically 8 or 12, but also up to 22 electrodes), is the solution initially developed by Dieter Gerlich in Chemnitz and widely used today. In figure 6.5d, the diagram of the PIIM double trap compares the radial potential created by an octupole trap and a quadrupole trap.

Fantasy For a demonstration trap, the most fanciful geometries are possible. A famous demonstration experiment showed that it is possible to trap charged particles in a paper clip, and specialists in high-voltage and high-frequency systems know that dust accumulates near circuits in organized structures.

We explained in paragraph 6.1 that it is not possible to trap ions with electrostatic fields alone. This statement is correct if trapping means stopping an ion at a given point in space. With an electrostatic field, it is however possible to trap an ion dynamically, *i.e.* to make it follow an almost closed trajectory around a set of electrodes. This is the technique used for the Zajfman trap, which consists of two electrostatic mirrors facing each other, or for the orbitrap developed by Alexander Makarov, which consists of two concentric electrodes around which the trajectories of the ions are wound.

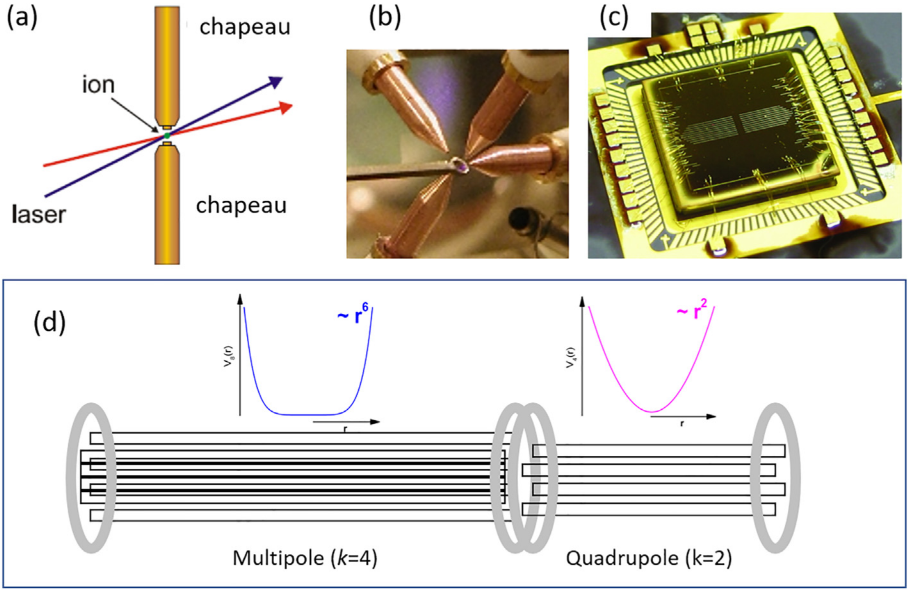

FIG. 6.5 – (a) Endcap (chapeau) trap (b) Ring trap (c) Surface trap developed for quantum information processing. (d) Octupole/quadrupole schemes (8/4 electrodes) and radial potential curves.

6.2 How to Cool Trapped Ions?

Now that we have explained how to create and store ions, we will look at their dynamics. We have to admit that our ions have no reason to be cold, and that they are surely very hot after a violent creation and under the effect of the trapping fields. The potential depth of the Paul or Penning traps is usually several eV (electron volts), an energy which corresponds to temperatures of the order of 12 000 K. In radiofrequency traps, the combined effect of collisions with the residual gas and the oscillating electric field is at the origin of the transfer of energy from the electric field to the motion of the ions, a phenomenon called radiofrequency heating. This effect leads to very hot ion clouds, so in order to carry out precision measurements it is essential to cool the ions.

The first method that comes to mind to cool the ions is to use a buffer gas, for example helium, which by successive collisions with the trapped ions and with the walls of the vessel containing the trap will bring their temperature into equilibrium with that of the walls. The ions can thus be cooled down to room temperature (300 K), to the temperature of liquid nitrogen (77 K) or liquid helium (4 K) with cryogenic devices. This technique is used for example for the characterization of heavy molecular ions, in particular of biological interest, such as peptides, or for the cooling of Hg^+ ions in the microwave atomic clocks that we will discuss later.

For high precision spectroscopy experiments, the presence of a buffer gas is not ideal. The collisions that occur will have an effect on the lifetime of the atomic levels and will therefore alter the atomic properties, not to mention the fact that helium is likely to form molecular ions with the ion under study (such as HeH^+) and therefore destroy the sample.

Laser cooling, a well known technique to obtain cold atoms (see chapter 1), was initially developed to cool atomic ions. Let us recall that the performances are excellent since laser cooling generally allows to reach temperatures of the order of mK (thousandth of a degree above absolute zero) for Doppler cooling and up to a thousand times lower using other more sophisticated laser cooling methods.

It should be noted that in ion traps, Doppler cooling is implemented with a single laser beam in a simpler way than for neutral atoms. Indeed, the oscillating movement of the particles and the Doppler effect tune the ion in resonance with the laser when it is directed against the laser, and out of resonance when it is directed in the same direction as it. It is then sufficient that the laser beam has a non-zero projection along each of the three directions of ion motion for the ions to be effectively cooled. The Doppler limit temperatures that are reached are of the millikelvin order for most of the ionic species studied today.

In their interaction with light, laser cooled ions undergo very many (5–40 million) spontaneous absorption–emission cycles per second. This gives a very convenient way to monitor the ions by imaging the fluorescence light on a CCD camera to see the ion cloud appear, as illustrated in figure 6.6.

One of the great interests of ion traps is the possibility of trapping several ion species simultaneously in the same trap. As the ions interact *via* the Coulomb force between their charges, it is sufficient to cool one of the ion species by laser for the other ions to be cooled. This is called sympathetic cooling. This technique is widely used today in laboratories, with the mythical ion pairs Be^+/Al^+ or Mg^+/Al^+ for aluminium ion optical clocks, and Be^+/H_2^+ or Be^+/HD^+ for molecular hydrogen ion spectroscopy and possible applications for antimatter creation.

Let us note that in the particular case of Penning traps, there are two other methods allowing to cool the ions efficiently to the temperature of the trap enclosure, *i.e.* between 300 and 4 K depending on whether the set-up is cryogenic or not. The first of these methods applies only to very light particles, such as the electron or its antiparticle, the positron, and is called radiative cooling. In the Penning trap, the charges make a cyclotron rotation around the magnetic field lines at frequencies of several GHz (billion revolutions per second). They undergo a very strong acceleration, and according to the laws of electromagnetism, radiate energy. Their motion is therefore naturally damped in a few seconds. The second method is called resistive cooling and applies to any ion in a Penning trap. The motion of the ions close to the trap electrodes induces an *image* current in the circuit connecting the electrodes. If this circuit has an electrical resistance at temperature T (usually 4 K), the interaction of the ion with the induced current leads to a dissipation of the kinetic energy of the ion, thus to its cooling.

6.3 Let Us Put Several Ions in the Trap!

Now that we know how to create, trap, and cool ions, we can try to put more of them in the trap. The question then is how many ions can a trap hold, and what will be the state of the ion cloud. Is it gaseous, liquid, or solid? Are new phases of matter possible?

Experiments show that it is possible to confine very large quantities of ions in a trap, the maximum quantity depending mainly on the size of the trap. Indeed, ions of the same charge repel each other and will not remain confined in the same place. It is the competition between this repulsion and the trapping force that forces the ions to stay together that determines the density of the ion cloud and its shape. The size of the trap then determines the total number of ions it can hold. The densities that can be realized are of the order of 10^{14}–10^{15} particles per m^3, which corresponds to an average distance between ions of 22–10 μm. A trap of centimetric dimensions can thus contain from a single ion to several million ions.

The distances between the stored ions depend on the confinement potential. The linear ion chain is a particularly interesting configuration because it allows the manipulation of each atom individually either by focused laser beams or by magnetic field gradients, which opens the door to the manipulation of quantum registers.

The structure of an ion cloud is determined by its temperature. At high temperatures, the cloud is in a gaseous state, it becomes liquid below a few kelvins and will crystallize at low temperatures (at temperatures of a few hundredths of a degree Kelvin) if Doppler laser-cooled. Indeed, an equilibrium between cooling, mutual repulsion of ions, and trapping potential allows to observe a very beautiful phenomenon: at the coldest temperatures, an ensemble of ions will arrange itself in stable structures and form quasi-crystals, like those visible in figure 6.6. In these pictures, each bright spot is the fluorescence of a single ion, which can be observed with a good camera. Figure 6.6 shows successively, from top to bottom, a single ion, a linear chain of ions, a cloud of a few thousand ions, and two clouds containing two species of ions. The second species, insensitive to the cooling laser, does not emit fluorescence and appears black in the figure.

There are cooling techniques to reach temperatures below the Doppler limit. They are only applicable to small numbers of ions, from one to a few units. In this case, a set of N ions behaves like a giant molecule and presents 3 N coupled modes of vibrations. It can be described by 3 N quantum harmonic oscillators. It is possible to prepare the system so that each of the associated harmonic oscillators is in its fundamental quantum state. This gives access to new states of matter, known as “entangled states”, where the dynamics of one ion is totally correlated to that of the other ions. These states are extremely important since they are the basis of quantum information processing, quantum simulations or quantum logic spectroscopy.

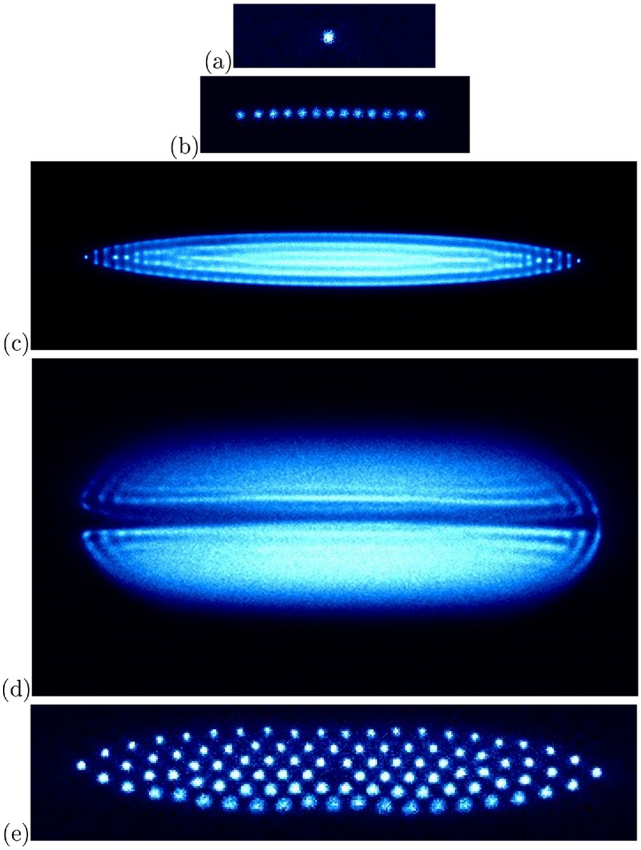

FIG. 6.6 – Fluorescence image of ion clouds obtained in the same trap, for different trapping configurations. (a) single Be^+ ion, (b) linear chain of 13 Be^+ ions, (c) crystal of a few hundred Be^+ ions, (d) mixed crystal containing Be^+ ions visible by their fluorescence and H_2^+ molecular ions that do not interact with the laser and appear black, (e) planar ion crystal containing 96 Be^+ ions and one H_2^+ ion. Typical distances between the ions are 10–20 microns. Images obtained by Thomas Louvradoux and Johannes Heinrich, PhD students at the Laboratoire Kastler Brossel at Sorbonne Université.

6.4 What can We do with Trapped Ions?

The very high control of the trapping parameters, but also the great ease of interrogation of the trapped ions, as well as the versatility of the traps that allow to confine as well a single ion as a million ions, explain the success of the traps in a large number of fields. In the following, we describe a small selection of examples where the use of an ion trap has opened up new routes.

6.4.1 Precision Measurements: Masses, Atomic Properties, ...

Mass spectrometry

Ion traps were originally designed as mass filters, and still play a prominent role in mass spectrometry today. Measuring mass *via* frequency is the approach of researchers using a Penning trap. The physics of Penning traps is a little bit more complicated than the description given above in the paragraph 6.1.1 presenting the Penning trap, the full description of the confinement dynamics of a single ion reveals a very accurate method of measuring the mass of this ion. Indeed, the apparently complicated trajectories can be decomposed into three simple and independent motions, the modified cyclotron motion which is a fast rotation of frequency f'_c close to the ideal cyclotron frequency and of small radius around the magnetic field lines, an axial harmonic oscillator motion of frequency $f_z = \frac{4qU}{2\pi m}$ in the z direction and a magnetron motion which is a slow rotation of frequency f_m around the Oz axis of the trap. The corresponding trajectory is shown in figure 6.2. A theorem states that the cyclotron frequency fulfils $f_c^2 = f_c'^2 + f_z^2 + f_m^2$. The precise measurement of these frequencies in a trap containing a single ion allows to determine the quantity $f_c = \frac{qB}{2\pi m}$ with 10, 11 and soon 12 significant digits! One could think that this is enough to determine mass m of the ion. Unfortunately, this is not the case because it is impossible to know the value of the magnetic field with such a precision. A clever solution is to successively trap two ions of different mass in the same magnetic field: mass ratios can be determined with an excellent precision and atomic and nuclear models can then be tested with the same precision.

Atomic properties

Each atomic or molecular species has its own energy levels. The absorption of one or more photons is possible if the energy of the photon or the photons is equal to the difference between two energy levels. The set of wavelengths of possible transitions in an atom or molecule forms its absorption spectrum, and a bit like a barcode, allows the identification of species. This is the purpose of spectroscopy, which has many applications: in astrophysics to optically identify elements present in stars or around planets, or in analytical chemistry for the comparison of samples, or the detection of traces for the fingerprinting of wines, or for doping controls, etc.

The very long trapping times combined with the interrogation by light of a well-defined wavelength, allow to excite in a very precise way atomic transitions between the energy levels of the ionic species studied. Using a time-resolved observation protocol where the fluorescence of the ions is monitored following a laser excitation phase, we can obtain the de-excitation curve of the atomic level and thus measure its lifetime. Further analysis allows to evaluate the branching rates, *i.e.* the relative probabilities of de-excitation from an excited state to lower energy levels, and to compare the results obtained with theoretical models of the ions. This technique can be extended to ion species that cannot be directly laser cooled using sympathetic cooling by a species of comparable mass. This has allowed the spectroscopy of the HD^+ isotope of the molecular hydrogen ion and comparison of the rotational or vibrational transition frequencies of this ion with *ab-initio* calculations up to 9 significant digits!

6.4.2 Strong Confinement Regime and Ion Clocks

The frequency resolution of spectroscopy experiments is often limited by Doppler broadening. The Doppler effect corresponds to the fact that the frequency of a sound or an electromagnetic wave perceived by a moving observer differs from the frequency measured in the source reference frame. Consequently, the width of the atomic resonance lines is often limited by the Doppler broadening, which can remain important (tens of MHz) even for ions cooled to the Doppler limit of a few mK.

Radio-frequency traps have an important advantage in eliminating the Doppler effect, an advantage that allows them to achieve incredible precision values: by well choosing the trapping potential, it is possible to constrain the oscillating motion of the ions in such a way as to reach very small amplitudes of motion. When this amplitude is less than a fraction of the wavelength of the probed atomic transition, the experiment enters the so-called strong confinement regime where the observed lines can only take certain values. They are no longer subject to Doppler broadening and have an ultimate spectral width given by the lifetime of the probed levels. This condition is easily met with a trap (and thus an ion cloud) of centimetre size for spectroscopy in the microwave range. This explains the success of radio-frequency traps for the very first mercury ion atomic clocks. Their development continues today for space applications because buffer gas cooling is sufficient to achieve excellent precision performances. In the optical frequency domain, the strong confinement regime can only be reached in the absence of micro-motion, *i.e.* with atoms confined where the oscillating electric field that creates the confinement of the ions is cancelled. In this case, the motion of the trapped ion is described by the model of the quantum harmonic oscillator, the one taught in the very first courses of quantum mechanics. There are cooling methods that allow to prepare the ion in the fundamental state of the harmonic oscillator and to reach the strong confinement regime. Most ion atomic clocks use a single ion (Yb^+, Sr^+ for example) confined in the center of the trap. The reproducibility and stability of these clocks are equal to those of the neutral atom clocks described in chapter 2, and reach frequency resolutions of 18 and soon 19 significant digits, that is to say the tenth of a second on the scale of the age of the universe!

Can we extend this method to ions which cannot be easily cooled by laser, but which can be interesting for precision measurements? The answer is yes, as shown by the aluminium ion clock developed in the NIST laboratories in the USA. In this case, a pair of Be^+/Al^+ (or Mg^+/Al^+) ions is confined in the same trap. The Coulomb repulsion between the two ions induces a coupling between their degrees of freedom so that we can no longer distinguish the motion of one of the protagonists from that of the other: this is what we call coupled oscillators. It is then sufficient to laser-cool the motion of the Be^+ (or Mg^+) ion so that the motion of the aluminium ion is automatically cooled, and to prepare the ion pair in its fundamental vibrational state. From there, a protocol called quantum logic spectroscopy is applied to probe the energy levels of the *spectroscopic* ion (here the Al^+ ion) by observing the *logic* ion (here Be^+ or Mg^+). Indeed, the law of conservation of the impulse indicates that the absorption of a photon resonating with a transition of the spectroscopic ion is accompanied by a recoil of this ion which takes the impulse of the photon. This changes the vibrational state of the ion pair, which is detected by analyzing the fluorescence of the ion. The total correlation between the internal state of the spectroscopic ion and the quantum vibrational state of the ion pair is called *quantum entanglement*.

This method is in fact very general, and several projects are trying to apply it to the spectroscopy of ionic species, in particular molecular ions that cannot be directly laser-cooled today. The developments it implies are closely related to those presented in the following paragraph for the control of quantum information.

6.4.3 Quantum Information and Quantum Simulations

Trapping and controlling individual atoms with great precision open the way to experiments on the manipulation of quantum information (see chapter 3). In a computer, a classical bit can take the values of 0 and 1 and with a large number of these basic modules the operations of the computer are implemented. Such a bit can be realized by an atom, and we can consider that the fundamental state $|0\rangle$ and the excited state $|1\rangle$ of the atom are the equivalents of the classical 0 and 1. Now, in an atom the quantum bit or qubit can take both values; but also any other linear combination between the two, and the state of the atom can be written in a two dimensional vector space as

$$|\Psi\rangle = \alpha \cdot |0\rangle + \beta \cdot |1\rangle$$

With their excellent control and ability to probe and manipulate individual atoms, trapped ions are therefore natural quantum bits. Furthermore, it is possible to design a quantum bus through the interaction of individual ions in particular with their vibrational modes in the trap.

The first demonstrations of quantum logic gates were made with small chains of 2 ions, but very quickly the question of scaling up the device to larger ion numbers has been raised. A real quantum computer must be able to handle hundreds of qubits and each proposed system must be evaluated on its capacity to integrate the largest number of qubits in the smallest possible volume. Concerning ion traps, a modular and extensible architecture has been proposed, based on the advances made in the field of micro-fabrication. Indeed, only traps of micrometric size allow to reasonably consider a multiplication of the number of qubits beyond a few tens of units.

One of the technical obstacles to the scaling up of systems is, among other things, the low robustness of the systems against decoherence (technical term related to the loss of information on the coefficients α and β appearing in the above equation). Atoms can be very easily perturbed by their environment, event interrogating the atoms by a laser to probe their state can disturb the measurement. Fortunately, in the traps, the ions communicate with each other, so we can trap two ions, ask questions to one and collect the answer about the state of the other. The best configuration is to choose two different species, so that the interrogating laser interacts only with a specific ion.

Despite intense research and some very promising experiments, the number of qubits that can be controlled is still very small. But the techniques and methods have already been implemented to pursue another path, that of quantum simulation (see chapter 4). The idea is to use a model system for a problem that is impossible to observe directly and difficult to explore by computation. This approach is interesting to model for example condensed matter systems, atom by atom.

6.4.4 Cold Collisions and Cold Chemical Reactions

The very long confinement time, and the fact that one can accumulate ions from an oven or a beam of atoms (or molecules) are the reasons for the success of the ion trap with the community of chemists and physical chemists. After adapting the geometry to their needs by choosing a multipole configuration, the trap has become a standard tool for studying (cold) collisions and chemical reactions.

The addition of cooling techniques, in particular laser cooling, allows to explore a wide range of sample temperatures and to record curves of reaction rates of species, very dependent on their energy. The preparation of atoms and molecules at very low temperatures and by the unit (see also the chapter 7) opens the way to the observation of individual chemical reactions without the thermal agitation of the particles masking their real behaviour.

6.4.5 Antimatter Confinement

Antimatter research has been an exciting area since the first theoretical postulates. Today, hydrogen anti-atoms are produced from anti-protons and positrons. The production of these two constituents is technically complex and requires specific sources which exist at CERN in Geneva. The particles produced are very energetic and to catch and keep the created anti-hydrogen, cooling techniques must again be used. The preparation of the elementary constituents is done with modified Penning traps, and the (neutral) antimatter can be held in a magnetic trap for times exceeding fifteen minutes. These exploits have already allowed the spectroscopy of anti-hydrogen atoms and prepare a future measurement of gravity to answer the still open question of whether an anti-atom falls like an atom under the effect of the earth's gravity.

6.5 Conclusion

You get the idea: ion traps are versatile and can be adapted to different situations and issues. We have chosen to present a few of the most followed axes, but we have not talked about the incredible applications such as the implementation of a heat engine cycle with a single ion or the implantation of ions one by one in a matrix for lithography, nor about one-component plasmas, large ion clouds that allow to simulate fundamental questions of plasma physics in an extremely well controlled system, let alone model systems for the Kibble–Zurek mechanism originally developed for cosmology or the interrogation of confined nanodiamonds. Some of these and more experiments are described in a recent specialized book edited by Martina Knoop, Niels Madsen, and Richard C. Thompson, entitled *Trapped Charged Particles* and published by World Scientific, Europe (2016).

For ion traps new avenues are constantly opening up, made possible by this simple ion cage that was designed for one initial purpose. The community of ion trappers is small but inventive, new ideas continuously add to the incredible number of experiments and applications that are possible with trapped ions!

Chapter 7

Cold and Ultracold Molecules

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What about extending the physics outlined in the previous chapters to molecules? Can molecules be cooled by laser? Then trapped? Are they useful for precision measurements, for quantum simulation, or for quantum information? Do they have their own applications? We will see in this chapter that the answer to all these questions is positive and that specific and original methods had to be developed to address them.

Arthur Leonard Schawlow, co-inventor of the laser and winner of the Nobel Prize in Physics in 1981, is credited with the famous quote: “a diatomic molecule is one atom too many!”. If atoms and molecules are two quantum systems with well-defined energy levels, this extra atom gives a molecule two extra degrees of freedom (vibration of the nuclei, rotation of the molecular axis) which, in the ultracold domain, immediately open new perspectives, richer than for cold atoms alone. Moreover, this extra atom makes the molecule a non-spherical object that can possess a permanent dipole moment that makes it very sensitive to an external electric field.

The manipulation of dipolar molecules by electric and magnetic fields allows novel studies such as the dipole–dipole interaction, the simulation of interacting spin systems, as well as the possibility to use molecular dipoles as supports for quantum computing. More broadly, ultracold molecules offer new possibilities of high-resolution spectroscopy or precision measurements such as fundamental studies of left–right symmetry (enantiomers), or concerning the variation of fundamental

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constants (mass of the proton, of the electron, Planck's constant h, etc.). The research field of cold quantum chemistry, with fully controlled reactions, becomes accessible based on perfectly prepared reactants in well defined initial quantum states and perfectly measured reaction products in final quantum states.

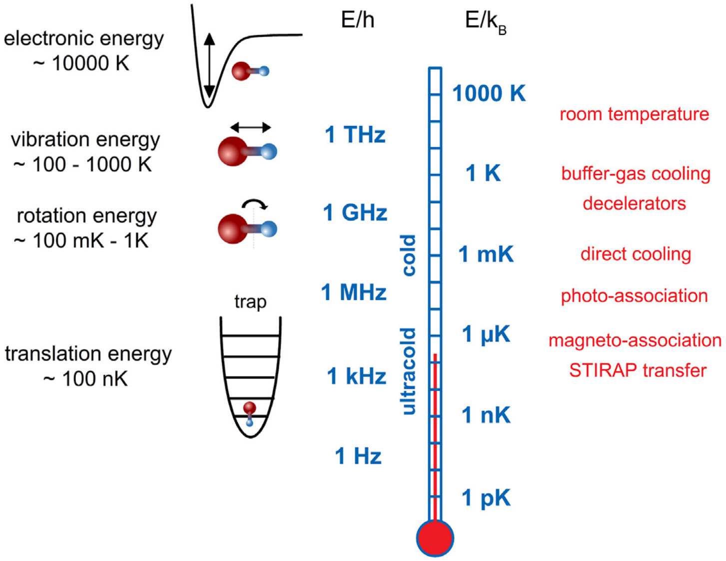

Fig. 7.1 – Energy scale E, also presented in units of temperature T (*via* the formula $E = k_B T$, where k_B is the Boltzmann constant) and frequency v (*via* the formula $E = hv$, where h is Plank constant) indicating, on the left, the typical orders of magnitude of the different degrees of freedom of a small molecule. On the right, starting from room temperature (298 K or about 25 °C), some methods that researchers have developed to lower the temperature of molecules are indicated, *i.e.* the energy of their translational motion.

A fundamental concept of molecular physics appears: the quantification of the energy of the different degrees of freedom illustrated in figure 7.1. The electrons move and turn rapidly around the nuclei, which oscillate (vibration) and rotate (rotation) while the whole molecule performs a translational motion in space. Here it is important to specify that when we speak about temperature, it is most often associated with the translational velocity, as for the atoms, and not with the internal motions (rotation or vibration) of the molecule.

The field of cold molecules started in 1998 when, almost simultaneously, two teams, one French and the other American, succeeded in producing molecules with a very low velocity. The French team of the CNRS (Laboratoire Aimé Cotton) located at the University of Orsay took the route of associating together two ultracold cesium (Cs) atoms previously cooled by laser, to form a molecule (Cs_2) that is ultracold in translation (microkelvin range). The American team from Harvard University designed a method for cooling an already existing molecule (calcium hydride: CaH) to reach so-called cold temperatures (millikelvin range).

The aim of this chapter is to explain how, since then, the research on cold molecules has experienced a vertiginous development by following these two parallel paths: (i) an indirect path by associating ultracold atoms, which unfortunately often forms vibrationally excited molecules (vibrationally hot), and which requires the implementation of optical techniques to attenuate the vibration of these molecules; (ii) a direct path by cooling molecules which unfortunately are often not yet slow enough. The two ways are currently merging and physicists are approaching the Holy Grail of this research field: to succeed in controlling each of the internal (electronic, vibration and rotation) and external (translation) degrees of freedom. We will start by giving some elements to understand the structure of a molecule, then we will explain why laser cooling techniques for atoms are not easily transposed to molecules. We will then detail the solutions that researchers have found to circumvent this problem. As it is often the case in research, this exploration has led to the emergence of initially unsuspected lines of study, such as a full controlled chemistry at ultracold temperatures, and the implementation of efficient measurement protocols to test the point-like nature of the electron or the mirror symmetry of matter.

7.1 How to Characterize a Molecule?

This simple question hides a great richness because the chemical bond is located at the border between classical physics and quantum mechanics. This has led to the development of different theories and experiments, based on the motion of atoms (nuclei and electrons) constituting the molecule, to understand its structure and its chemical reactivity.

7.1.1 The Electronic, Vibrational, Rotational Energy Levels

A molecule, an assembly of two or more atoms, is a system much more complex than an atom. Indeed, a molecule is no longer a spherical object: in addition to the motion of electrons around the atomic nuclei, there are internal degrees of freedom, namely the vibration and rotation of the nuclei. If the molecule is made of two different atoms, its electron cloud presents an asymmetry giving rise to a permanent electric dipole moment which favors the interaction of the molecule with an external electric field.

This assembly of electrons (of total mass m) and nuclei (of mass M at least 2000 times greater than that of the electrons) in mutual interaction is characterized by an energy scale for each of its internal motions (figure 7.1): the electrons motion, characterized by energy E_{el}, the vibrational motion, characterized by energy E_{vib} and the rotational motion of the nuclei, characterized by energy E_{rot}. These energy scales verify the ratios:

$$\frac{E_{\mathrm{vib}}}{E_{\mathrm{el}}} \approx \frac{E_{\mathrm{rot}}}{E_{\mathrm{vib}}} \approx \sqrt{\frac{m}{M}}. \tag{7.1}$$

Thus, this ratio is about 0.01 for $^{7}\mathrm{Li}_2$, and 0.002 for $^{133}\mathrm{Cs}_2$, two emblematic molecules of the ultracold molecule domain. Figure 7.2 shows these levels for the ground state and an excited state of $^{133}\mathrm{Cs}_2$. By associating frequency ν (by $E = h\nu$), and thus characteristic time $1/\nu$ to these energies (figure 7.1), we deduce that the rotation is slow ($\sim 10^{-10}$ s) compared to the vibration ($\sim 10^{-12}$ s), which is itself slow compared to the electron motion ($\sim 10^{-15}$ s).

It follows that in a first approximation, one can decouple the fast motion of the electrons from the slower motion of the nuclei. This view was first justified and formalized in 1927 by the physicists Max Born and Julius Robert Oppenheimer, who proposed a simplified solution of the Schrödinger equation. This is to fix the distance R between nuclei A and B of a diatomic molecule, and to calculate the electronic energy $E_{\mathrm{el}}(R)$ and wave function $\psi(R)$ corresponding to each quantum state of the system. The knowledge of wave function $\psi(R)$ gives access to all the properties of the molecular system; in particular, the square of its norm $|\Psi(R)|^2$ is related to the probability of presence of the two nuclei at the considered distance R. This calculation is repeated for each distance R, which is equivalent to considering that the fast electrons adapt immediately to the change of position of the nuclei: this is called an adiabatic approximation.

Energy curves $E_{\mathrm{el}}(R)$ are called potential energy curves, or potential curves. For R very large, the molecule dissociates, and the potential energy joins the sum of the energies of the considered atomic levels called dissociation limit. On the contrary, when R becomes small, $E_{\mathrm{el}}(R)$ becomes infinitely large, reflecting the Coulomb repulsion between the nuclei. The state with the lowest electronic energy is called the ground state, and the other states with higher electronic energies are the excited states. The molecule is stable if $E_{\mathrm{el}}(R)$ has a minimum at distance R_e called the equilibrium distance. It is necessary to provide an energy at least equal to $D_e = E_{\mathrm{el}}(R = \infty) - E_{\mathrm{el}}(R_e)$ to dissociate molecule AB into its two atomic constituents A and B. Each potential energy curve is different (different values of equilibrium distance, dissociation energy, curvature…).

As its name suggests, $E_{\mathrm{el}}(R)$ is the potential energy generated by the rapid motion of the electrons, and is the energy the nuclei are subject to, whose motion is then quantized. When a given electronic state is associated with a potential curve having a minimum energy, vibrational energy levels characterize the oscillating motion of the nuclei. In addition, each vibrational level is superimposed with rotational levels: we speak of rovibrational levels. Finally, as for an atom, a molecule can have an electronic spin and a nuclear spin which can give rise to other energy levels called fine or hyperfine. Thus, to fully characterize the state of a molecule, we will give its electronic state (*e.g.* a singlet state for a null electronic spin or a triplet state for an electronic spin equal to 1), its vibrational state v and its rotational quantum number j.

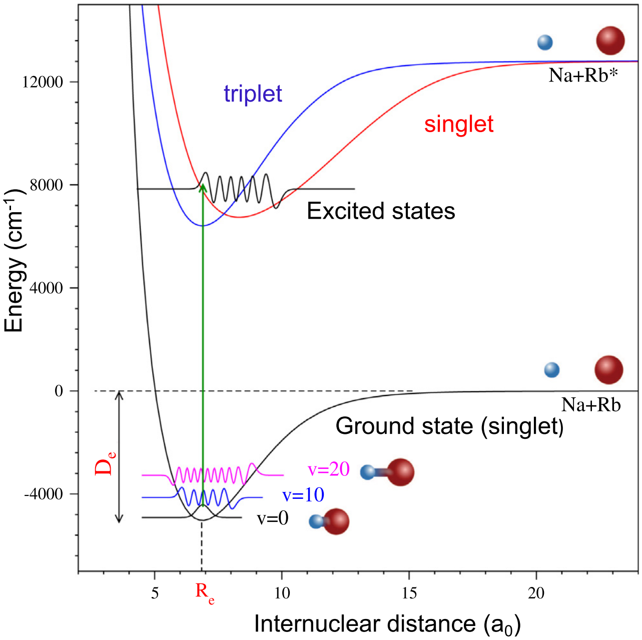

FIG. 7.2 – Potential energy curves of the ground state and excited states of the NaRb molecule as a function of the distance between the Na and Rb nuclei. The ground state tends to the dissociation limit where the two separated atoms Na and Rb are in their ground state. The equilibrium distance R_e is the distance where the molecule is most stable. Dissociation energy D_e is the energy that must be supplied to the stable molecule to dissociate it. Also, schematically shown are the wave functions associated with the vibrational levels $v = 0$, $v = 10$ and $v = 20$. The gap between the rotational levels is too small to be visible at this scale. The excited potential curves tend towards the dissociation limit corresponding to Na in the ground state and Rb in an excited state. According to the Franck–Condon principle (see §7.1.2), the most efficient transition from the $v = 0$ vibrational level of the singlet ground state is represented by a green arrow, which connects it to a vibrational level of the singlet excited potential (zero electronic spin), which is accessible according to the electronic selection rule from the ground state (while transitions to the triplet excited state, of electronic spin 1 are forbidden).

It happens that two potential curves cross at distance R_c, indicating that the electronic energy of two different states is the same at this distance. The Born–Oppenheimer approximation above is then no longer valid, since the nuclear motion (of the nuclei) can then abruptly change at this distance. The calculation of the rovibrational levels of the molecule must then include simultaneously the two curves in question. This remark is not anecdotal: indeed, it is this type of phenomenon that is at the origin of chemical reactions, *i.e.* the transformation of molecular species into each other. Without this break in the Born–Oppenheimer approximation, chemistry, and therefore the world as we know it, would not exist!

7.1.2 Can We Laser Cool Molecules?

Probability of transition during absorption or emission of photons: Franck–Condon principle

To complete this presentation, we must study the interaction of a molecule with light. Just like the possible transitions (absorption or emission of photons) of an atom, the transitions between electronic states of a molecule are governed by selection rules reflecting in particular the fact that the photon has an angular momentum equal to 1 (in units of the reduced Planck's constant $\hbar = h/(2\pi)$). Thus, the absorption or emission of a photon can only occur if the orbital angular momentum of the electron that absorbs, or emits the photon, changes by one unit. Only transitions between states, whose angular momentum changes by one unit, will therefore be possible. This implies that quantum number J associated with the total angular momentum of the molecule (including its rotation and the total angular momentum of the electrons) will only vary by one unit at most during a photon absorption or emission. The spin of the electron, being sensitive only to the magnetic field and not to the electric field created by the photon, does not change in this process. The transitions will therefore not be possible between a singlet electronic state and a triplet electronic state.

It is important to note that because the vibrational motion is not concerned by angular momentum, vibrational transitions are not restricted by a strict selection rule. Vibrational quantum number v can therefore change strongly when a photon is absorbed or emitted, the efficiency of this process being governed by the so-called Franck–Condon principle. Figure 7.2 shows an example of the application of this principle where the most favorable transition from the $v = 0$ vibrational level of the ground state occurs towards the $v = 12$ level of the excited state which is accessible by the electronic selection rules.

To demonstrate this important principle, one must compare the characteristic time of electronic transitions following the absorption or emission of a photon (~ 1 fs) to the characteristic time of a structural re-organization of atoms ($\sim 1 - 100$ ps). The Franck–Condon principle stipulates that these vibrational transitions take place without the nuclei having time to move, *i.e.* at fixed internuclear distance R. These are the so-called vertical transitions (figure 7.2). In quantum mechanics, this is expressed using the probabilities $|\mathbf{\Psi}_{\text{vib},1}(R_1)|^2$ of finding the system at position R_1 at the beginning and $|\mathbf{\Psi}_{\text{vib},2}(R_1)|^2$ at the same position R_1 at the end of the transition. More precisely, the transition probability between the vibrational states 1 and 2 is given by what is called the Franck–Condon factor $\left|\int \mathbf{\Psi}^*_{\text{vib},1}(R)\mathbf{\Psi}_{\text{vib},2}(R)\,dR\right|^2$. This factor represents the overlap between the wave functions before and after the absorption of the photon and governs the intensity of transitions between vibrational levels of a molecule. A transition between vibrational levels is therefore intense if the two vibrational wave functions involved in the transition overlap constructively (*e.g.* the left lobe of the excited wave function in figure 7.2 overlaps with the lobe of the wave function of $v = 0$).

Why is it difficult to laser cool molecules?

The internal degrees of freedom and the dipole moment that molecules possess make them ideal candidates for many applications, provided that they can be cooled and a dense sample can be obtained in a well-defined quantum state, ideally in the lowest ground state energy, which is still a real challenge today.

The idea that comes up spontaneously to cool molecules is to use the same laser techniques as those developed to manipulate, cool and trap atoms, techniques that rely on the existence of a radiation pressure force applied by light on atoms (see chapter 1). This force is the result of an exchange of photons and therefore of the transfer of momentum between an atom and a light wave during cycles of absorption and spontaneous emission. As explained in chapter 1 of this book, to exert such a force on an atom, we shine it with a laser beam, resonant with a transition between its ground state level and an excited level. The efficiency of this force is directly related to the existence of a closed or nearly closed optical transition (figure 7.3), *i.e.* such that the spontaneous emission occurs predominantly towards the initial level of the transition. Indeed, if during the absorption-spontaneous emission cycles an atom is transferred to a state other than the initial one, resonance with the laser frequency is not ensured anymore and the radiation pressure force disappears. In the case of figure 7.3a where the leakage occurs towards a very small number of levels, repumping lasers that bring the atom back to its original state after an absorption–emission cycle can be added to solve this difficulty.

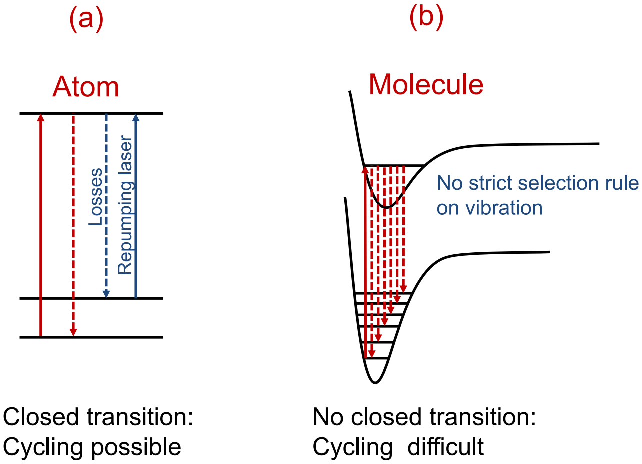

Fig. 7.3 – The efficiency of direct laser cooling relies on the existence of a closed or quasi-closed optical transition, *i.e.* such that spontaneous emission (red dotted arrow) occurs practically only towards the initial state of the transition. In the case of an atom (a), the losses by spontaneous emission (blue dotted arrow) towards a level other than the initial level of the transition are compensated by means of a laser called repumping. In the case of a molecule (b), the losses occur towards a large number of vibrational levels because the vibrational transitions are not governed by strict selection rules, preventing a sequence of a large number of optical cycles.

A molecule, in a given electronic state, has a large number of vibrational levels. However, as we have seen in the previous paragraph, vibrational transitions are not governed by strict selection rules. This lack of selectivity is problematic for optical cycling because most excited molecules relax easily in several vibrational levels. The population of each of these levels is given by the Franck–Condon factor between the initial and final levels (figure 7.3b). To recover these lost molecules, it would be necessary to set up as many lasers as there are leakage levels, which makes the realization of a laser cooling experiment of molecules very complex.

In 2004, Michael Di Rosa developed the idea of laser cooling of a subset of diatomic molecules which present favorable Franck–Condon factors (close to 100% between only 2 levels) and which have indeed been cooled by laser like SrF, CaF, CaH, YO, etc. This method will be described in more detail in paragraph 7.3.3.

7.2 Associating Cold Atoms

An alternative to laser cooling of molecules is the formation of ultracold molecules from atoms previously cooled by laser. This approach, called “indirect”, allows to associate pairs of ultracold atoms during their collisions, without changing the motion of the center of mass, thus preserving the translation temperature of the atoms. However, the produced molecules have in general a high internal energy of vibration and rotation that must be eliminated by other techniques. The ultimate goal is to obtain a dense sample of molecules in a well-defined quantum state, ideally the absolute ground state, *i.e.* in the lowest electronic, vibrational, rotational (and possibly hyperfine) energy levels.

7.2.1 With a Photon: Photoassociation

Photoassociation consists in exciting a pair of free atoms in collision (A and B) towards a bound level of an excited state of the AB^* molecule. By adequately choosing this excited state (by maximizing the Franck–Condon factors of the involved transitions), one can promote de-excitation by spontaneous emission towards certain bound vibrational levels v of the ground electronic state of the AB molecule. The process

$$A + B + \text{photon}_1 \rightarrow AB^* \rightarrow AB(v) + \text{photon}_2$$

is illustrated in figure 7.4. This technique allowed the team of Laboratoire Aimé Cotton (LAC) to produce for the first time cold Cs_2 molecules in 1998. The final translation temperature is close to the initial temperature of the cold atom cloud (typically in the microkelvin regime). The photoassociation followed by spontaneous emission allows to reach bound levels of the ground electronic state of the molecule, but these have a high vibrational energy because the de-excitation is governed by the Franck–Condon principle: the levels reached are those whose overlap with the bound level of the excited state is significant. However, the energy of the populated vibrational levels can, by inelastic collisions with the other molecules or the residual atoms of the gas, be converted into kinetic energy and thus increase their

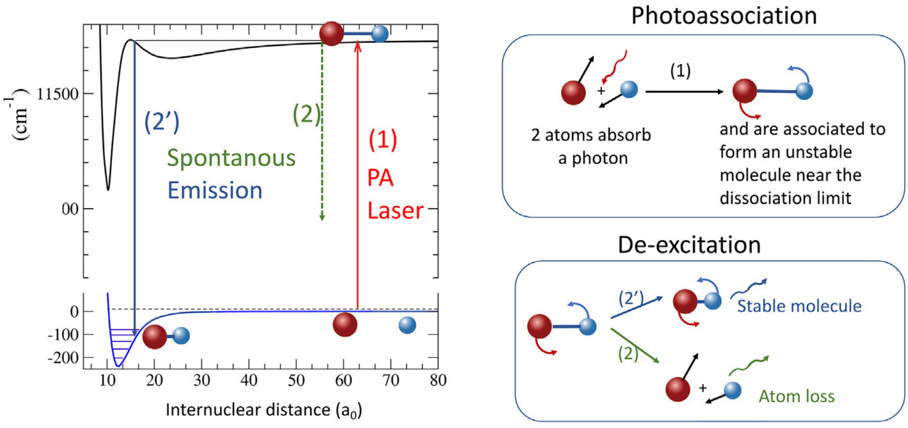

FIG. 7.4 – Illustration of the association of atoms by absorption of a photon followed by the de-excitation of the molecule thus formed. The process is presented on the right and explained by the Franck–Condon principle (overlapping wave functions) on the left. A pair of free atoms absorbs a laser photon in a process (1) called photoassociation (PA) to form an electronically excited molecule. The Franck–Condon principle implies that the molecule is formed in a vibrational state close to the dissociation limit. It is therefore natural that the reverse process (2) of emission of a photon to (re)form two dissociated atoms is very likely. However, by inducing an excitation towards a well chosen potential curve, like the one here that presents a double well, it is sometimes possible to increase the presence time of the two atoms at shorter internuclear distances and to favor the process (2') of de-excitation by spontaneous emission towards ground state levels of the molecule.

temperature, which can cause escape of molecules from the trap. These limitations of photoassociation led the LAC team to develop vibrational and rotational (re) pumping techniques in order to gather the whole population of molecules in a single vibrational and rotational level of the electronic ground state.

7.2.2 With a Magnetic Field: Magnetoassociation

The association of two cold atoms A and B can also be realized with the help of a variable magnetic field according to the reaction

$$A + B \overset{\text{magnetic field}}{\longrightarrow} AB$$

This magnetoassociation technique relies on the possibility of adjusting Feshbach resonances (also described in chapter 4) by means of the magnetic field. These resonances, sometimes also called Fano-Feshbach resonances, were introduced independently by Ugo Fano and Herman Feshbach at the end of the 1950s, in their work on atomic and nuclear collisions, respectively. A Feshbach resonance occurs when, in a collisional process, a bound state of the molecule AB is coupled with the free state of the colliding pair of atoms A and B. The effect of the coupling is strong when the energy difference between this bound state and the free state is close to zero, *i.e.* in the case of resonance.

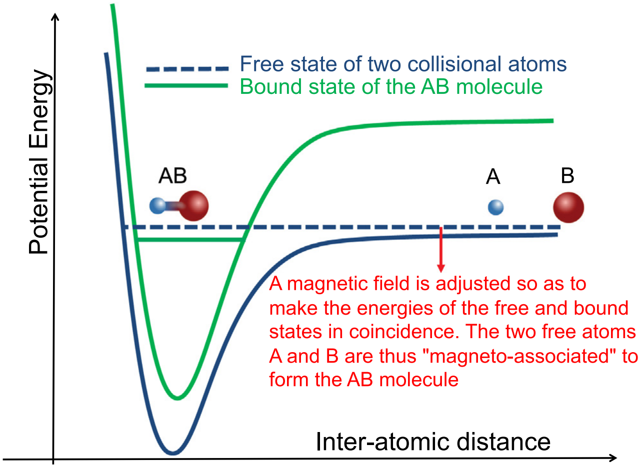

FIG. 7.5 – Two free cold atoms A and B are in collision in a free state of an electronic state. A magnetic field is used, the intensity of which is carefully varied so as to bring the energy of this free state into coincidence with that of a bound state of molecule AB: this produces what is known as a Feshbach resonance, which allows to transfer the pair of cold atoms to a bound level of an electronic state of the molecule and to form a cold molecule. This process of association of two atoms is called magnetoassociation.

The experimental principle, illustrated in figure 7.5, consists in slowly changing the value of the magnetic field to modify the effect of the interaction by slightly shifting the potentials until the energy of the free state of the colliding atoms coincides with that of a bound state of the molecule, in other words, until a resonance occurs, allowing the stabilization of the colliding atoms in a bound vibrational state of the molecule.

7.2.3 How to Control Association?

In both cases of photoassociation or magnetoassociation, the formed molecular sample keeps the initial temperature of the gas of atoms, *i.e.* a temperature much lower than the millikelvin. However, the molecules obtained are in high vibrational levels of the electronic ground state, and thus possess a high internal energy. Transferring the population of these high levels to the ground state (lowest energy level) of the molecule is the major challenge of many ongoing experiments. An efficient method uses a two-photon transfer from an initial level (the high vibrational level) to a final level (the ground state level), relying on a well chosen intermediate level. This process is achieved by means of a sequence of laser pulses where the first pulse couples the final state to the intermediate level while the second pulse couples the same intermediate level to the initial state, as described in figure 7.6. It can be shown that using this somewhat counter-intuitively order of pulses, this transfer called STIRAP (STImulated Raman Adiabatic Passage) allows the coupled molecule-photon system to follow an evolution where the population in the excited intermediate level remains constantly zero, thus avoiding losses induced by spontaneous emission. This formation method allows to obtain ultracold molecules in their ground electronic and rovibrational state, and has been successfully used by many groups on Cs_2, Rb_2, KRb, RbCs, NaRb, NaK molecules.

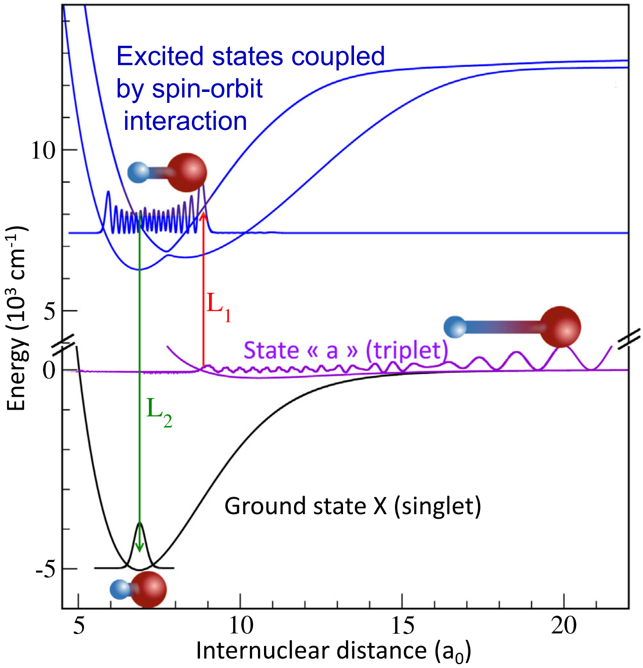

FIG. 7.6 – Illustration of the population transfer by two laser pulses according to the STIRAP (STImulated Raman Adiabatic Passage) method in an ultracold molecule. The molecule is initially prepared in the triplet state (purple) by magnetoassociation of atoms and is transferred to the singlet symmetric ground state X (black). A direct transfer is forbidden by the electronic selection rules. This transfer uses as intermediate states the two excited states of singlet and triplet symmetry (in blue) which cross each other and which mix their characters by an interaction, called spin–orbit interaction, which confers a singlet and triplet character to the vibrational wave functions of these mixed states. The triplet part of the wave function allows to excite the molecules from the initial triplet state, while the singlet part of the wave function allows the transfer to the X state. The efficiency of the transfer depends on the intensity of the absorption (red arrow) and stimulated emission (green arrow) lines, determined by the intensity of the lasers and the overlap (Franck–Condon factor) of the initial and final wave functions with the wave function of the intermediate state.

7.3 Direct Cooling of Molecules

Although the formation of cold molecules by association of cold atoms is efficient, it is nevertheless limited to molecular species made of atoms that can be cooled by laser, *i.e.* alkali-metals (*e.g.* Rb, Cs...), alkaline earths (*e.g.* Ca, Sr…), rare gases (Ar, Kr…) and lanthanides (Yb, Dy…). Therefore, this method is not suitable for the formation of cold molecules consisting, for example, of oxygen or carbon atoms. It is then natural to consider a direct cooling of the molecules. As it is outlined in chapter 1, atoms can be cooled to less than one kelvin by dissipating their translational energy. Moreover, even when considering only Doppler cooling, a large proportion of atoms are in the electronic ground state because of the short lifetime of the excited state. Subsequently, this makes Bose–Einstein condensation accessible for atoms. For molecules, the situation is much different. If some cooling techniques may cool the translation of molecules, the vibrational and rotational motions are not necessarily frozen. For example, in a cooling technique based on refrigeration, *i.e.* where the molecules are in contact with a cold gas, the vibration and rotation levels are populated by collisions. Note also that, in a gas of cold or ultracold molecules, black body radiation at room temperature can also modify the population distribution of the internal levels of the molecule.

A cooling process of molecules is said “direct” when it does not rely on the laser cooling of the atomic compounds. Here, the objective is to cool molecules formed at high temperatures ($T > 300$ K). As no method is currently available to directly cool molecules from high temperatures to the ultracold regime, it is necessary to proceed in several steps. The first is to form molecules and cool them at a temperature of a few kelvins through a thermalization process involving a cold source. All the techniques used to achieve this step lead to form a molecular beam. It is very important to understand that these molecules are cold (typically in the kelvin or sub-kelvin range) in a reference frame that moves at the average velocity of the beam. The task consisting in slowing such a beam is a second stage. The molecule decelerators developed to this end are generally based on electromagnetic forces. Once the molecules are slow enough, a third step can be implemented to reach the sub-millikelvin regime.

7.3.1 Formation and Preliminary Cooling

To cool a gas of molecules available at room temperature or formed at higher temperatures, refrigeration is an efficient method. It requires a thermal contact between the molecules and a cold source of noble gases (He, Ar, Ne, Kr, Xe). The choice of a noble gas is linked to its very low chemical reactivity with the molecules. These gases are cooled to temperatures of 1–10 K thanks to two techniques that should be distinguished. The first one consists in cooling the noble gas initially at room temperature by an adiabatic expansion; the molecules in the gas are then cooled together with the noble gas. With the second technique, the noble gas is previously cooled to a cryogenic temperature (4–20 K) before being brought into contact with the molecules.

Supersonic beams cooled by adiabatic expansion

In a cooling experiment using an adiabatic expansion, a noble gas is initially contained in a high-pressure chamber (0.1–100 bars), at a temperature of $T = 100$–300 K. By expanding the gas in a vacuum chamber, a cooled atomic beam can be formed. For example, with a standard argon expansion, the beam velocity can reach the supersonic velocity, at about 550 m.s^{-1}, and a temperature of ~ 1 K. Optimized devices are able to give temperatures of the order of 10 mK.

Molecular cooling by expansion requires to put the molecules in the buffer gas. For this, there are several techniques whose choice depends on different criteria, such as the stability or the physico-chemical properties of the chosen molecular species. Direct mixing of the molecules in the buffer gas is surely the simplest approach. When this is not possible, the molecule can be formed by chemical reaction or laser ablation of reactants, or by dissociation of parent molecules.

The collisions with the buffer gas act on the external (translation) as well as internal (vibration, rotation) degrees of freedom. The efficiency of molecular cooling can be characterized through effective temperatures T associated with each degree of freedom, in the sense of a population of an energy level E in proportion to the Boltzmann factor $e^{-E/(k_B T)}$. It appears that the larger the energy separation between the internal states, the more the efficiency decreases. This is for example what we observe with monofluorides molecules (BaF, CaF, YbF) which are produced in excited states by laser ablation: typically, the translation temperature is $T_{\rm trans} \approx 1 - 10$ K, the rotation temperature is $T_{\rm rot} \approx 10 - 30$ K and the vibration temperature is $T_{\rm vib} \approx 1000 - 10000$ K.

Effusive beams cooled by cryogenic refrigerators

The cryogenic cooling technique discussed here takes place in a chamber, called a cold chamber, of a few tens of cm^3 cooled by a refrigerator to a cryogenic temperature of 1–20 K. The noble gas (or buffer gas in this context) that is introduced into it is cooled by contact with the walls, and finally extracted to a vacuum chamber through an orifice. The flow of the gas in the vacuum follows a so-called effusive beam regime whose temperature is approximately the same as in the cold chamber. Its velocity is about 100 m/s. The introduction of the molecules in the cold chamber can be done by a fine pipe (capillary pipe) or, if the molecule is not stable, by its formation *in situ.* The thermalization of the molecules with the buffer gas in the cold chamber is reached after about a hundreds of collisions. The molecules are then dragged into the beam.

Compared to supersonic beams, effusive beams based on cryogenics allow to cool a larger number of molecular species and are also significantly slower than in the supersonic case. This last point is very advantageous when considering slowing down the molecular beam.

7.3.2 Deceleration of Molecular Beams

The sample of cold molecules obtained by supersonic expansion or by cryogenics moves at a velocity in the range of 80–600 m/s. At this stage, the objective is to slow down the beam of molecules until a sample at rest is obtained in the laboratory frame. With this deceleration technique, the study of collisions at low energies as well as trapping become accessible. For this purpose, many techniques have been developed over the last twenty years. We will only detail here the most widespread systems, namely the Stark decelerators and the Zeeman decelerators (here the Zeeman decelerator is of a different design than the Zeeman decelerator mentioned in chapter 1, designed for an atomic beam).

The kinetic energy of molecules can be decreased using the interaction between their electric or magnetic dipole and an external electric or magnetic field: for a molecule in a given quantum state, the interaction results, respectively, in an energy shift called Stark shift (for an electric field) or Zeeman shift (for a magnetic field). Decelerators are devices that create inhomogeneous fields along the propagation axis of the molecular beam, thus inducing a spatially modulated energy shift. Based on this principle, there exist different approaches that are able to achieve efficient deceleration. We present here the most common decelerator (sequential decelerator) illustrated by figure 7.7. This type of decelerator has a periodic structure composed of identical segments aligned on the axis of the beam; these segments are pairs of electrodes (Stark decelerator) or coils (Zeeman decelerator). The global deceleration of the beam means that the molecules lose a part of their kinetic energy as they pass through each segment: as they pass through a segment, the interaction potential energy with field (ΔE_p) increases. According to the principle of conservation of total energy, kinetic energy E_c necessarily decreases. For $\Delta E_p \ll E_c$, velocity v decreases by quantity $\Delta v \approx v\Delta E_p/(2E_c)$. For a total rest of the beam, it is thus necessary to cross many segments whose number is estimated by $N \approx E_c/\Delta E_p$. This schematic process requires some practical corrections. First of all, we have to take into account the dispersion in velocity and position of the molecules in the beam. For this reason, the molecules do not pass through each segment under the same conditions, and some of them are subject to possible instabilities, or worse, to acceleration. Another important point is the guidance in the axis of the decelerator. Since the structure of the field respects Maxwell's equations, the segments necessarily produce forces transverse to the propagation of the beam; the molecules are thus likely to leave the decelerator by the edges. These decelerators are mostly adapted to light molecules. Moreover, they are inefficient for non-polar molecules (without electric dipole) or molecules not sensitive to the magnetic field (diamagnetic molecules) such as N_2.

Other types of decelerators have been proposed and even tested with success; however, although ingenious in design, their use is to date rather marginal. One example is the "centrifugal" decelerator where the molecules, introduced in a rotating electrical guide, lose their kinetic energy in the form of centrifugal potential energy. Another approach uses two crossed beams of gas; one of the two contains the molecules which, after collisions with the atoms of the other beam, mechanically lose their kinetic energy. It is also possible to realize a beam from a rotating nozzle; the rotation velocity is adapted to compensate the beam velocity, leading to an arbitrarily slow beam in the laboratory frame. Finally, there are optical methods based on pulsed lasers delivering high peak intensities; it has been demonstrated that these lasers are able to produce sufficient conservative optical forces for effective deceleration.

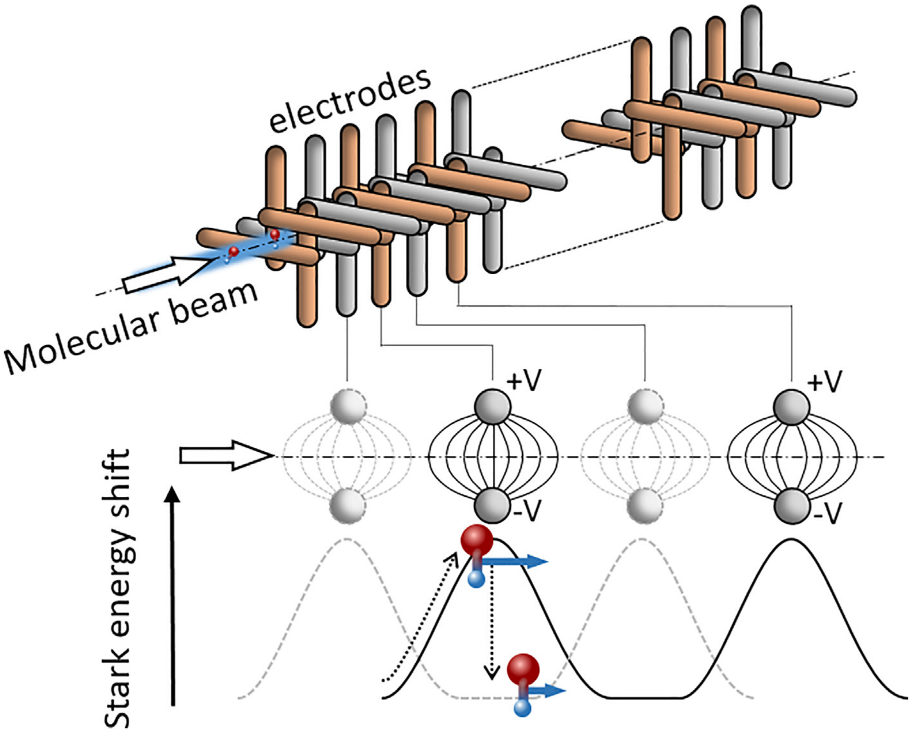

FIG. 7.7 – Electric field deceleration (Stark decelerator). The device is formed by a succession of pairs of identical electrodes centered on the axis of the beam of molecules. When a pair of electrodes is brought to a potential V, it creates an electric field interacting with the molecular electric dipole. When a molecule passes between two electrodes and its interaction potential energy increases, its kinetic energy decreases accordingly. This process being reversible, the electric potential must be quickly turned off when the loss in velocity is maximum. The succession of such sequences, by playing on the on and off switching of the pairs of electrodes, allows the beam of molecules to be slowed down. The lighter the molecules, the more efficient the slowing is.

7.3.3 Sub-Kelvin Cooling

The methods described above do not enable to reach ultracold temperatures, and the search for methods capable of filling the gap between the millikelvin and microkelvin range remains an important area of research. We have already discussed the fact that laser cooling of molecules raises some problems because of the internal degrees of freedom — rotation and vibration — that can be excited by the transfer of momentum of a photon during spontaneous emission. Thus, a molecule in an electronically excited state typically de-excites in several vibrational levels of the electronic ground state (figure 7.3b). This means that many lasers (repumping lasers) are needed to keep the molecules from absorbing photons. For laser cooling to be possible, an important idea was proposed in 2004 and realized in 2010: one must choose suitable molecular species, ideally molecules for which the Franck–Condon factor of the laser cooling transition is close to 100%. This means that the vibrational wave functions involved in the transition must be almost identical: this is the case when the shapes of the electronic potential energy curves are very similar, within the same distance range. In other words, if the molecule has an electron which plays a insignificant role in the molecular bond, then the structure of the molecule is barely modified during the excitation of this electron by the cooling laser. This can be achieved, for example, using an alkaline earth metal atom (Mg, Ca, Sr, Ba,..) linked through a simple ionic bond with an electronegative binding partner, such as fluorine (F). The s^2 valence electron configuration of the alkaline earth indeed allows an ionic bond: one of the s electrons creates the bond, while the other remains localized on the atom. This electron can be excited by strong optical transitions, like the $s \rightarrow p$ transitions used in the laser cooling of alkali atoms. This intuitive picture highlights why molecules like fluorides, hydrides or monoxides (SrF, CaF, CaH, YO...) are good candidates for laser cooling. These molecules have all been cooled to date and, in 2014, the first magneto-optical trap of molecules was even realized with SrF by a team at Yale (USA). In order to avoid a heating up of the rotation, it is necessary to perform an excitation that reduces the total angular momentum of the molecule ($j \rightarrow j-1$), in contrast with the $j \rightarrow j+1$ case for atoms. This leads to experimental complications: for example, it is necessary to quickly and synchronously invert the polarizations of the trapping lasers and the gradient of the applied magnetic field. The capture of molecules from cold beams described above is rather limited and the number of molecules remains currently low ($\approx 10^5$) with limited densities ($<10^{14}$ per m^3), but the temperatures can reach the sub-Doppler regime of about tens of μK.

A very promising line of research concerns polyatomic molecules. Indeed, "pseudofluoride" molecules with an electron that participates only weakly in the bonding, such as a valence electron on non-bonded orbitals ($CaCH_3$, $MgCH_3$, SrOH, YbOH), must be able to be cooled by laser. A team from Harvard in the USA, pioneer in this research, cooled by laser in 2017 the SrOH molecule, and in 2020 those of CaOH and $CaOCH_3$. The technique could work with much larger molecules (such as hydrocarbon radicals), which would offer unique capabilities to conduct interdisciplinary research in physics, chemistry and even biology. In general, these methods would allow to use a Y radical, chosen for the physico-chemical properties we want to study, to attach it (for example in SrO–Y) to a quasi isolated system where laser cooling is possible.

Another method of cooling is the so-called Sisyphus method. Here it is a matter of converting kinetic energy into potential energy using external forces. In the field of cold atoms, where the concept of Sisyphus cooling mentioned in the preface emerged, the potential energy is created by light potentials. The idea here is to generalize this concept, initially proposed by David E. Pritchard in 1983, using electric or magnetic potentials. The idea is ultimately very similar to the one used in the Stark or Zeeman decelerators: it is necessary to repeat sequences of loss of kinetic energy (this is called Sisyphus cooling, a character from Greek mythology, condemned to push a stone to the top of a mountain from which it always ends up falling back). The fundamental difference is the use of a spontaneous emission step that returns the molecule to its original state. The advantage of this method, demonstrated using an electrostatic trap by a German group in 2012 on fluoromethane (CH_3F), then in 2016 on methanal or formaldehyde (CH_2O), is that at each step the loss of kinetic energy can be very large, of the order of several mK, to be compared to the loss related to the recoil of a photon, on the order of μK during a standard laser cooling. The method is thus general and very efficient because the cooling requires only a few hundred cycles, which makes the technique less sensitive to losses in states outside the cooling cycle. If the method can be applied with purely rovibrational transitions, it is obviously possible to combine this method with a conventional laser cooling method. This research area opens the possibility to exploit laser forces based on coherent processes by multiphoton momentum transfer which are more efficient, as it has been investigated on SrOH.

Finally, a promising method is the cooling using collisions with dense and colder species, such as atoms or ions cooled by laser, in a so-called “sympathetic” cooling scheme. Such thermalization technique has been explored for molecular ions, with for example, in 2009 the cooling to 150 mK of a biomolecule (glycyrrhetinic acid: $C_{30}H_{46}O_4$) in a crystal of barium atomic ions. Sympathetic cooling of neutral molecules with trapped ions also seems possible although reactivity and inelastic collisions severely limit the efficiency of the process currently.

7.4 Cold Molecules: For Which Applications?

The methods we have just described allow to form cold molecules in well defined internal states, in particular the absolute ground state. What can we now achieve with these cold and stable molecules? What are the applications of these systems and what are their advantages compared to atoms? The main difference is that the particular arrangement of the molecules gives them specific properties that neutral atoms (in the electronic ground state or in a highly excited electronic state such as the Rydberg states introduced in chapter 4) or atomic ions do not have. Let us take for example the simplest case of a diatomic molecule: in its own body frame, this molecule has a cylindrical symmetry unlike a single atom which is spherically symmetric. If the diatomic molecule is heteronuclear, *i.e.* composed of two different atoms, the molecule has in its body frame an intrinsic electric dipole moment oriented along the molecular axis. When an electric field is applied, the average value of this intrinsic electric dipole moment, which is called the induced electric dipole moment d_{ind}, takes a positive or negative value along the electric field in the laboratory frame, as illustrated in figure 7.8. If the induced electric dipole moment is positive, it is directed in the same direction as the electric field, and in the opposite direction if it is negative.

Fig. 7.8 – When electric field $\vec{E}$ is applied in the laboratory, electric dipolar molecules acquire on average an induced electric dipole moment d_{ind}, along the electric field. The most electronegative atom, *i.e.* the one which tends to attract the shared electrons of the molecule, is represented by a blue sphere, and the least electronegative by a red sphere. We thus associate a net charge + on the red sphere and − on the blue sphere. This defines the orientation of the induced electric dipole moment, from the − charge to the + charge. The value of this moment is positive if it is directed in the same direction as the field (left molecule), and negative if it is directed in the opposite direction (right molecule).

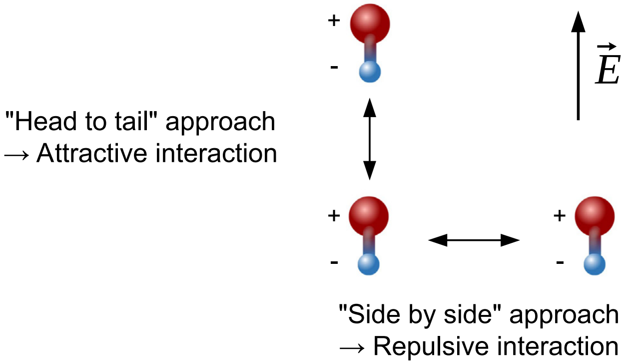

Fig. 7.9 – The electric dipolar interaction between two molecules is a long-range interaction, whose intensity is tunable by electric field $\vec{E}$, and strongly anisotropic. For example, a head-to-tail approach leads to an attractive interaction: the − charge of the upper molecule is attracted by the + charge of the lower molecule. A side-by-side approach leads to a repulsive interaction: the + charges of the left and right molecules repel each other, as do the − charges.

Two molecules can interact through the interaction between their dipoles. This is called dipole–dipole interaction or simply dipolar interaction. This interaction is strongly anisotropic and depends on the positions of the molecules: when the dipole approach is head-to-head, the dipolar interaction is attractive, whereas when the approach is side-by-side, the dipolar interaction is repulsive (figure 7.9). Moreover this interaction has also a very long range which can reach micrometers depending on the chosen dipolar molecules and the applied electric field. We must compare this distance with the average distance between two molecules in a gas. As an example, densities n reached in ultracold molecular gases are on the order of $n \simeq 10^{12}$ molecules per cm^3, and the average distance between two molecules is on the order of $n^{-1/3} \simeq 10^{-4}$ cm, that is on the order of the micrometer. Molecules can therefore interact and communicate at great distances without even colliding! When the range of the interactions is as large (or even larger) as the average distance between the molecules, we enter a special regime where macroscopic and collective quantum effects are important and where correlations between the particles appear (see chapter 4). Finally, the strength and the range of the interaction are tunable with the value of the electric field applied in the laboratory. It is thus possible to go from an uncorrelated regime at low field to a correlated regime at high field. All these characteristics make the richness of ultracold molecules. They are suitable candidates for applications such as quantum simulation, quantum information, ideal ultracold and controlled molecular chemistry experiments, and tests of fundamental physics.

7.4.1 Quantum Simulation

The precise control of the internal states (rotation, vibration) of ultracold molecules and their interactions as well as of their external states (translation) can be used to artificially engineer all kinds of quantum edifices, in particular in optical lattices. Optical lattices (see chapter 4), created by counter-propagating laser beams, form a set of localized sites that can trap molecules. Figure 7.10 illustrates the example of dipolar molecules in electric field $\vec{E}$ and in an optical lattice. Such lattice can be designed in one, two or three dimensions (see chapter 4). These setups are controllable and tunable: one can control the electric fields and their orientations (and hence the orientation and strength of the induced dipole moments of the molecules), the depth and spacing of the sites of the optical lattice by playing, respectively, on the intensity and the frequency of the lasers, and the inter-site interactions of the molecules, as illustrated in figure 7.10. The tunneling effect between two sites can also be controlled, allowing or not a molecule to be in the same site as another molecule. Therefore, intra-site interactions (and therefore collisions) can also occur. From this set-up, one can simulate the physical conditions of another system, such as electrons in a crystalline solid. One can thus imitate its behavior (more precisely its Hamiltonian, a quantity in quantum mechanics which characterizes the energy of all the possible states) by the simulator system, composed of the molecules in the lattice, much more flexible and tunable than the physical system itself. This is the idea of quantum simulation (see chapter 4). By analogy, the induced dipole moment d_{ind} of the molecules, pointing in the same direction as the electric field or in the opposite direction (see figure 7.8), plays the role of the $\pm 1/2$ components of the electron spin, the dipole–dipole interaction plays the role of the interaction between spins, and finally the optical lattice plays the role of the crystal lattice, made of positive ions. Molecules can move from one site to another by tunneling just as electrons can.

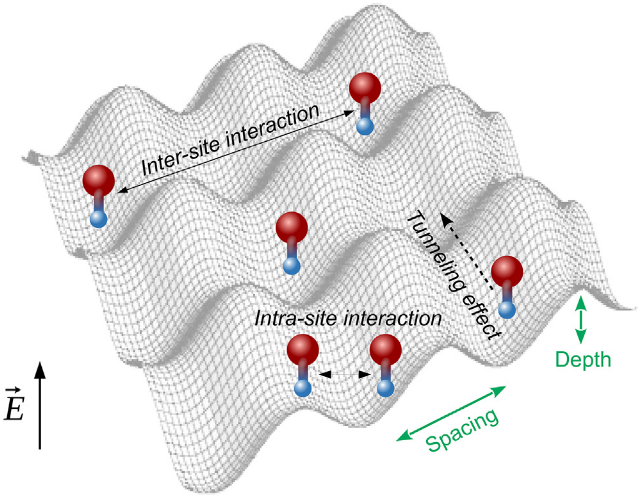

FIG. 7.10 – Dipolar molecules subject to electric field $\vec{E}$ and trapped in an optical lattice, created by counter-propagating laser beams. By adjusting the electric field and the spacing and depth of the lattice sites, we can control the strength and orientation of the interactions between the molecules. The distance between two sites is on the order of 0.5 μm. Depending on the chosen dipolar species, the electric field and the frequency of the lasers, inter-site interactions can occur at very long distances, on several sites. A molecule can move in the lattice by tunneling between two sites and eventually collide with another molecule present (intra-site interaction). These quantum edifices allow to simulate theoretical models, including strongly anisotropic models, to explain phenomena of condensed matter, especially crystalline solids.

These devices of quantum simulation could play a major role in the understanding of quantum phenomena such as superconductivity, quantum magnetism (ferromagnetic and anti-ferromagnetic orders in materials), superfluid and supersolid states, and quantum phase transitions. The simplest theoretical models developed to understand these phenomena can thus be reproduced by the simulator system. As for neutral atoms, the use of molecules allows to simulate a rich variety of Hamiltonians of systems, including those not accessible to condensed matter physics. Moreover, it is possible to realize all kinds of anisotropic models, thanks to the strongly anisotropic electric dipolar interactions (see figure 7.9). Finally, electric dipolar molecules interact through long distances, *i.e.* over several sites of the optical lattice. The use of molecules for quantum simulation thus offers wide possibilities, complementing those identified with neutral atoms (see chapter 4).

7.4.2 Quantum Information

The physical design of a quantum computer requires the realization of quantum logic gates, elementary operations acting on a small number of qubits, generally on one and two qubits (see chapters 3, 4 and 6). These gates are the basis of the circuits involved in quantum information processes. The qubits are represented by a superposition of quantum states, often denoted $|0\rangle$ and $|1\rangle$, carried by the atoms, ions or molecules. For an operation involving a two-qubit quantum gate, fast interactions between the two qubits are required. Moreover, the storage of qubits requires to identify stable long-lived states. Decoherence processes, created by the interaction between qubits and the environment or between two qubits, must be as small as possible.

Ultracold electric dipolar molecules offer all these advantages and are therefore a promising platform for the realization of these processes. Indeed, they can be produced in large quantities (like atoms), they interact strongly at long distances (like ions), and have a very long lifetime because the relevant spontaneous emission rates are low. In molecules, there are different quantum states that can be used as the basis state $|0\rangle$ and $|1\rangle$ to encode qubits, such as vibrational, rotational, or hyperfine states carried by the nuclear spin of molecules. This latter case is illustrated in figure 7.11, where we chose molecules in two well-defined hyperfine levels of the rovibrational level $(v = 0, j = 0)$ of the fundamental electronic state: such a state satisfies the condition of high stability or long lifetime.

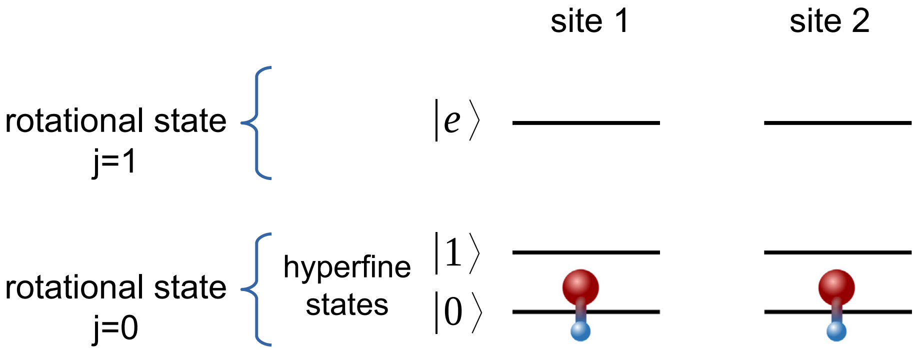

FIG. 7.11 – Example of quantum states of molecules used as basis states to encode qubits. Here, we have chosen molecules in their fundamental electronic, vibrational $(v = 0)$ and rotational $(j = 0)$ states. In the fundamental rotational level $j = 0$, we choose two hyperfine levels denoted by $|0\rangle$ and $|1\rangle$, carried by the nuclear spin of the molecules. These are the states that encode the qubits. For a quantum gate between two qubits, two molecules are on a site 1 and a site 2, for example in an optical lattice. A hyperfine state in the excited rotational state $j = 1$ of the molecules, denoted by $|e\rangle$, is also identified to realize a quantum gate.

7.5 Ultracold and Controlled Molecular Chemistry

When two molecules collide, different processes can occur. Let us take the simple example of a diatomic molecule AB in its fundamental electronic state, composed of two atoms A and B, characterized by the vibrational v and rotational j quantum numbers. During a collision between two AB molecules denoted 1 and 2, several types of processes can occur. We distinguish the non-reactive processes

$$AB(v_1, j_1) + AB(v_2, j_2) \rightarrow AB(v'_1, j'_1) + AB(v'_2, j'_2), \tag{7.2}$$

where the chemical identity of the AB molecules is preserved after the collision. The quantum numbers (v_1, j_1) and (v_2, j_2) correspond to the initial quantum states 1 and 2 of the AB molecules, and the quantum numbers (v'_1, j'_1) and (v'_2, j'_2) to the final quantum states. Elastic collisional processes are those for which the molecules do not change quantum states after the collision, so that $v'_1 = v_1, j'_1 = j_1, v'_2 = v_2, j'_2 = j_2$. Inelastic collisional processes are those for which at least one of the above quantum numbers has changed its value after the collision. When the chemical identity of the AB molecules is not preserved after the collision, it is referred to as a reactive process or a chemical reaction, such as:

$$AB(v_1, j_1) + AB(v_2, j_2) \rightarrow A_2(v'_1, j'_1) + B_2(v'_2, j'_2) \tag{7.3}$$

where molecules AB after the atoms rearrangement became molecules A_2 and B_2, with totally different chemical properties. In this case, the initial molecules are often called reactants and the final molecules are called products. Other products can be involved as trimers: $AB + AB \rightarrow A + AB_2$, or $AB + AB \rightarrow B + BA_2$. Note that for bi-alkali molecules in their absolute ground state, these trimer products are not energetically allowed.

The fine and precise study of these processes is the basis of what is called ultracold controlled chemistry. The ultracold temperatures reached in the experiments allow to consistently and accurately prepare all molecules of an ultracold gas in the same well-defined initial quantum state. In addition, some experiments start to measure the final quantum states of the molecules after the elastic and inelastic collisions of the reactants or the products of the chemical reactions. This determines the state-to-state transition probabilities from the well-defined initial quantum state to the measured final quantum state. These experiments manage to even detect the presence of intermediate A_2B_2 tetramers when the two AB diatomic molecules are close enough to each other so that they form a transient tetra-atomic complex. The presence of these complexes is important and demonstrates a certain pathway of chemical reactions. This is illustrated in figure 7.12. The experimentalists prepare the AB reactants in well defined quantum levels (this can be for example their ground electronic, vibrational and rotational states). The molecules approach during the collision until they reach the region of the tetra-atomic complex (black arrow) where the four atoms interact. After collision and depending on the paths taken, the collisional process can lead either to an elastic or inelastic process $AB + AB$ (red arrow), or to a reactive process $A_2 + B_2$ (green arrow). In each case, the molecules end up in rovibrational quantum states that are measured in the experiment with some probability. For example $P_{1\rightarrow 2}$ determines the probability of going from two molecules AB in the initial quantum state 1 to two molecules A_2 and B_2 in the final quantum state 2. It is the interactions that occur in the region where the four atoms are close to each other that are responsible for the paths taken by the

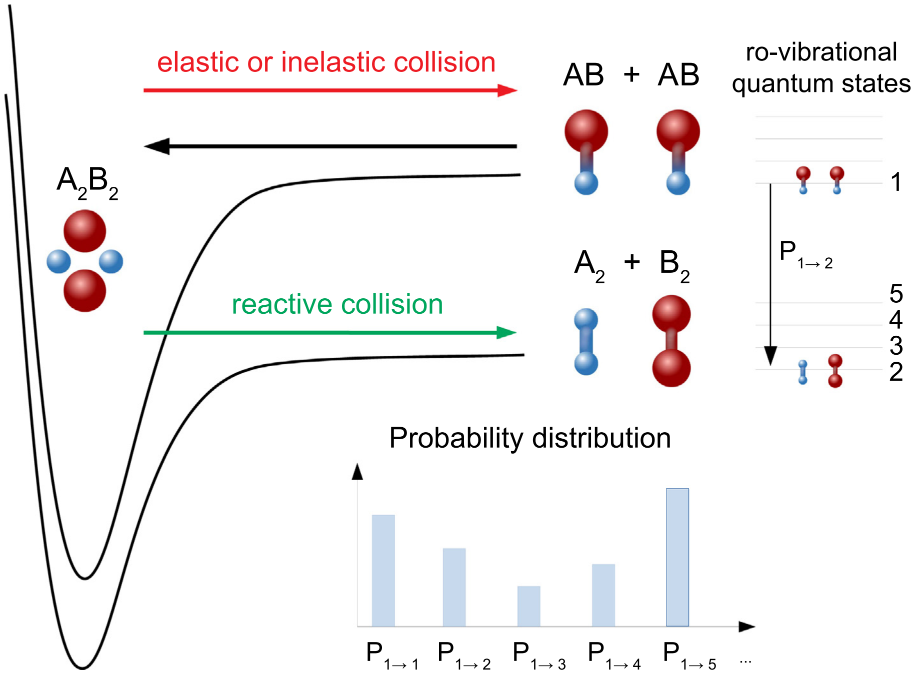

FIG. 7.12 – Schematic illustration of an ideal ultracold molecular chemistry experiment. An ultracold gas of AB molecules in a well-defined initial rovibrational quantum state is prepared (quantum state 1 on the right of the figure). Two AB molecules approach each other during the collision until they reach the region of the tetra-atomic complex A_2B_2 (black arrow) where the four atoms interact with each other. After collision, the collisional process leads either to an elastic or inelastic process $AB + AB$ (red arrow), or to a reactive process $A_2 + B_2$ (green arrow). The population of the final rovibrational quantum states is measured in the experiment, leading to a characteristic state-to-state probability distribution (bottom). Using different control methods such as electric and magnetic fields, electromagnetic waves or optical lattices of different geometries, one can modify this distribution of states at will: this is the principle of an ultracold and controlled molecular chemistry experiment.

atoms of the complex. They are responsible for the transition probability between the initial and final states. These experiments provide very valuable information about how a chemical reaction occurs. A chemical reaction can finally be fully controlled by different methods such as electric and magnetic fields, electromagnetic waves, or through the geometry of the collisional approach of reactants guided by optical lattices, in addition to temperature. All these tools of control can change the probability distribution of a chemical reaction and allow to engineer the final distribution at will. One can enhance or suppress one or many quantum state-to-state transitions of a chemical reaction according to a wanted final result: this is the principle of an ultracold and controlled molecular chemistry experiment.

7.5.1 Precision Measurements

Cold molecules, like cold atoms, can be used in high precision measurement experiments to test possible extensions of the Standard Model of fundamental physics (see chapter 2). The rich internal structure of molecules as well as their permanent electric dipole moment can thus be exploited for precision measurements such as that of the electric dipole of an elementary particle such as the electron, even though the electron is a point particle without structure. This may seem contradictory since an intrinsic dipole results from a non-spherical charge distribution. However, theoretical physics proposes that this intrinsic dipole of the electron appears due to complex interactions with other fundamental particles. The Standard Model of particle physics predicts a non-zero electric dipole moment d_e but its value is too small to explain the mysteries of particle physics such as the preponderance of matter over antimatter in the universe. Alternative theoretical models to the Standard Model (supersymmetry, string theory,...) predict an intrinsic electric dipole moment of the electron much larger than that of the Standard Model, which could then answer the problem of the matter/antimatter asymmetry. To reveal such a dipole, metrological experiments based on cold molecules offer the best measurements realized so far. The best current measurement uses a valence electron of the ThO molecule. One approach is to detect the energy shift $(-d_e E_{\text{eff}})$ induced by the interaction between intrinsic electric dipole d_e and electric field E_{eff} felt by this electron. Since the value of d_e is very small, we need the strongest possible electric field to induce a measurable energy shift. The electric fields that can be produced in the laboratory frame (typically on the order of 10 kV/cm) are not sufficient to modify these energy levels in an appreciable way. On the contrary, in the body frame of a molecule, the chemical bond strongly modifies the electronic energy. An electron inside a dipolar molecule feels a large effective electric field directed along the molecular axis, as illustrated in figure 7.13. For example, this field can reach values of $E_{\text{eff}} \simeq 100$ GV/cm in the ThO molecule. It is this enormous electric field that the electron feels that facilitates the measurement of a possible energy displacement $(-d_e E_{\text{eff}})$ linked to the dipole of electron d_e. It is then sufficient to measure the difference $(2d_e|E_{\text{eff}}|)$ between the energy given by one orientation of the field and that given by the opposite orientation, to deduce a value of d_e.

Another example is the measurement of the time variation of fundamental constants, such as the ratio m_p/m_e between mass of the proton m_p and that of the electron m_e, or the fine structure constant α. Let us take the example of ratio m_p/m_e. If its value changes over time, then the fact that the nuclei of atoms have protons implies that ratio m/M in equation (7.1) and therefore the ratios $E_{\text{vib}}/E_{\text{elec}}$ and $E_{\text{rot}}/E_{\text{vib}}$ must change as well. This change in the energy ratios of the different internal degrees of freedom of the molecules would be easily observed if two molecular levels had the same energy. Such a situation often occurs in molecules because they have a very rich variety and hierarchy of energy levels (electronic, vibrational, rotational), of different orders of magnitude, suitable to produce particular levels degeneracies. Therefore, the slightest change in these energies ratios would be observed by a lifting of the degeneracy of these molecular levels and a visible energy gap in the spectra that would change over time.

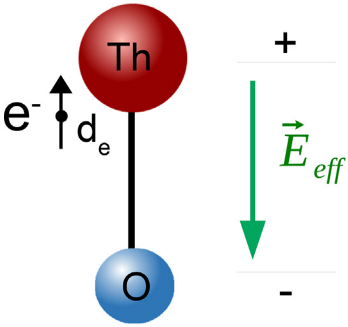

FIG. 7.13 – Principle of the measurement of the electric dipole moment of the electron d_e. In the thorium monoxide molecule (ThO), a valence electron of the thorium atom represented schematically, feels an effective electric field $E_{\text{eff}} \simeq 100$ GV/cm created by the covalent chemical bond between the Th and O atoms. The energy levels of the ThO molecule will thus be modified by an amount $-d_e E_{\text{eff}}$ that one has to measure. As the value of d_e is very small, an electric field as intense as possible is needed to detect it. Such a field is not possible in the laboratory frame but can be effectively produced in the body frame of a dipolar molecule (here $\simeq 100$ GV/cm): this is the reason to use this kind of molecule for such measurement.

Finally, a last example is that of chirality in biology which is, as underlined by the magazine Science for its 125th anniversary, one of the great scientific questions remaining unanswered. A chiral molecule has two enantiomer states (states that are images of each other in a mirror, with opposite rotational behavior): a levorotatory state (with left-handed rotational behavior) and a dextrorotatory state (with right-handed rotational behavior). It appears that nature favors mostly levorotatory amino acids and dextrorotatory sugars. This mystery could find an explanation similar to that proposed for the asymmetry between matter and antimatter, namely a symmetry violation of the Standard Model which would confer two different energies to the two types of enantiomers. This difference in energy being very small, it requires an extreme precision to measure it, that only cold (chiral) molecules could reach.

7.6 Conclusion

We showed in this chapter that cold and ultracold molecules are formidable tools leading to many original studies. Due to the richness of their numerous rotational and vibrational levels, or to the existence of a permanent electric dipole moment, they obviously offer more possibilities than atoms to study fundamental quantum effects — which makes them essential for precision measurements —, for simulation and quantum information or for the study of controlled chemistry. The counterpart of this richness remains in the challenge of their production as well as their manipulation by electric and magnetic fields, lasers or during collisions. Despite these difficulties, the ingenuity of researchers has allowed over the years to develop different techniques to reach a quasi-total control of many molecular species. These results guarantee that cold and ultracold molecules will remain a hot topic for a long time.

Chapter 8

Conclusion and Everything Else This Book Could also Have Been About…

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The chapters in this book have tried to give you an idea of the advances in physics that are due to gases cooled to extremely low temperatures. This field of research, to which the scientific community in France has largely contributed since its beginnings, has undergone a very important worldwide development in four decades. Every ten years, it has been completely renewed by unexpected discoveries and has exploded in different directions. This book is far from covering all the on-going work and many more developments could have been included. Each chapter is written by active researchers, who wanted to give you an idea of the richness of their domain, with examples particularly noteworthy in the field they are exploring together with their team. The authors of this book are betting that the scientific momentum given to their field will go on for long. But are we not about to reach a saturation of the ideas implemented by this research community? In this concluding chapter we hope to share with you our conviction that this is not the case. New concepts are continuously developed in laboratories, applications derived and perfected, as well as daring experiments are undertaken that no one could have imagined at the time when quantum mechanics was born. Here we will mention some topics that you have not heard about in this book and outline some new avenues of research with ultra-cold quantum gases.

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Alfred Kastler, the inspiration for the field

To begin with, let us recall that the field of very low temperature quantum gases emerged as a result of decades of research in atomic physics, moving beyond the stage where atoms are observed with light to the point where light manipulates them. A key step in the emergence of cold atom physics was optical pumping, for which Alfred Kastler was awarded the Nobel Prize in 1966: the preparation of the internal states of atoms by optical pumping is the basis of the magneto optical trap (MOT), as well as of the Sisyphus effect which explains why the cooling of atoms exceeds the limits initially expected (see preface). It should also be remembered that Alfred Kastler was the first to predict that a light field can decrease the temperature of an atomic vapor (see chapter 1) by the effect he called "lumino-frigoric" in a forgotten paper of 1950. In this book we would like to pay special tribute to Alfred Kastler (figure 8.1) for his pioneering work, not forgetting that after the war he was the founder of the laboratory at the ENS which now bears his name (Laboratoire Kastler Brossel). This laboratory was the historical birthplace in France of a whole generation of researchers involved in the field of cold atoms, such as Claude Cohen-Tannoudji, Jean Dalibard, Christophe Salomon, Alain Aspect and many others whose work is mentioned in this book.

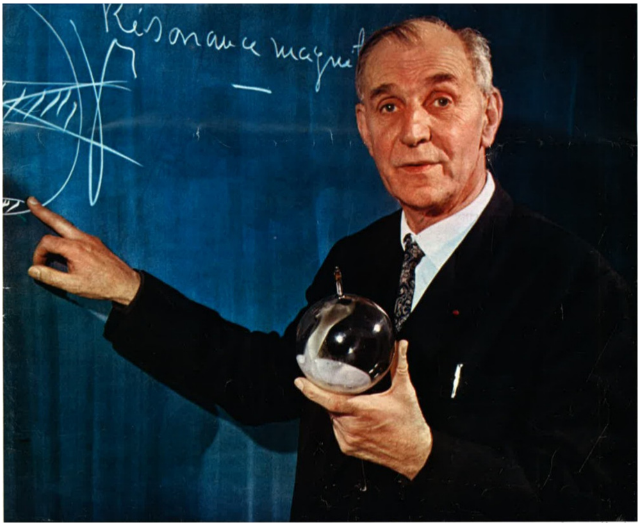

Fig. 8.1 – Alfred Kastler demonstrating to students with a sodium vapor in his laboratory at the École normale supérieure. He was awarded the Nobel Prize in Physics in 1966 for his work on optical pumping, which also involved his long-time collaborator Jean Brossel. Photo credit: Charles Courrière, cover of Paris-Match (12 November 1966).

More accurate clocks, more robust sensors for space

It should also be remembered that Alfred Kastler was already convinced in the 1950s of the importance of atoms for the definition of time. He quickly understood the strategic importance of atomic clocks, which replaced the old astronomical measurement methods with ever-increasing accuracy. From the 1960s onwards, he was able to observe the spectacular progress made in atomic clocks with the arrival of the laser. Too soon gone, he was unable to witness the spectacular progress following the use of cold atoms for such instruments. We can bet that he would have been amazed by the today achievements: the saga of this race for precision is told in chapter 2. Yet the story of clocks is far from over. Optical clocks with cold atoms trapped in a lattice, which today beat all records (drift of less than one second over 30 billion years, a period longer than the age of the Universe!), have certainly not yet reached their limits. They are competing for accuracy with the ion clocks described in chapter 6. In addition, the use of squeezed states of radiation described in chapter 3 opens the way to a reduced noise and thus to an improved accuracy for atomic clocks, as well as for other measurement instruments described in chapter 2. The use of cold molecules, rather than cold atoms, is also mentioned in chapter 7 as a promising trend. Another avenue under development exploits Dicke's states to realize new super-radiant optical clocks, in which the coherence properties are recorded in the collective atomic states rather than in the light inside a Fabry–Perot cavity. What will be the last word on precision for time measurement? Some believe it will go with nuclear clocks, where the reference will be a transition frequency of the nucleus of an atom or ion, *i.e.* higher than for the electronic transitions used in atomic clocks: accuracy would be increased, as well as robustness and stability. The research is focused on the nucleus of the thorium 229 atom, although the wavelength of the UV laser needed to operate the clock is not yet sufficiently specified. This highly multidisciplinary exploration is being carried out by a European consortium for which cooling and ion trapping methods are central.

Practical and theoretical importance of metrology

One may ask why such an endless push to improve clocks, which today are already by far the most accurate instruments ever built by man? In fact, metrology has always been of crucial importance for practical life and for economic and commercial relations between countries. The system of primary units of time, length and mass is periodically revised and internationally fixed. The primary unit of time, the second, follows the accuracy improvement of atomic clocks. Such instruments, as well as the interferometric sensors described in chapter 2, are expected to become more miniaturized, more robust and less expensive. Thus, a new generation of hybrid cold atom inertial sensors is being developed, integrating on the same chip the magnetic and optical elements necessary for the operation of the atom trap. This effort correlates with missions aiming at mapping the Earth's gravitational field from space. The applications of such instruments will grow more and more.

In a more theoretical field, high-precision spectroscopy makes it possible to test the fundamental laws of physics. One of the best confirmed theory is quantum electrodynamics (QED), which is increasingly questioned with ultra-cold atoms: the measurements provide values of fundamental constants with up to 11 significant digits, such as the α fine structure constant of atomic physics (see figure 8.2). The confrontation of experiments to one another and to the theory still creates passionate debates and sometimes brings surprises, such as for the recent well-publicized "anomaly" of the proton radius, questioning the foundations of the QCD theory (quantum chromodynamics). We have also seen how rich is the spectroscopy of ions in chapter 6, whether they are cooled by laser or indirectly by sympathetic cooling. Progress in precision is expected, coupled with progress in theory. We here recall the use of ultra-cold ions for the preparation of anti-hydrogen, the spectrum of which will be compared with that of hydrogen. The spectroscopy of cold molecules also has great potential to answer basic questions, such as: does the electron have an electric dipole moment (see chapter 7)?

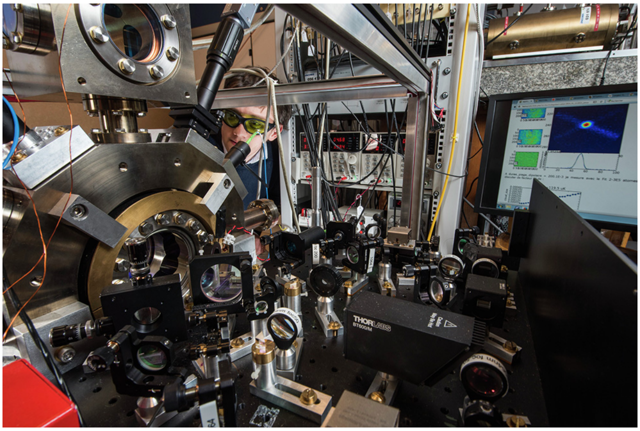

FIG. 8.2 – Arrangement for measuring the recoil of a rubidium atom as it absorbs a photon. In the vacuum chamber (left), laser beams are used to cool rubidium atoms. These atoms are then trapped by laser: on the right on the computer screen the image of the trapped atoms. This experiment aims at a very accurate measurement of the fundamental constant α at the basis of atomic physics. Photo credit: Hubert Raguet/Laboratoire Kastler Brossel/CNRS Photothèque.

Many candidates for quantum information

In the current development of quantum technologies, the very high level of precision that cold gases bring to metrology is undoubtedly their most advanced and most directly applicable feature. However, it is less of a public dream than the field of quantum information, which is still largely in progress but very promising. This field has been triggered by the advance of the founding experiments in cavity quantum electrodynamics, of which those of Serge Haroche's team are the most elaborate example. Chapter 3 shows how purely quantum phenomena give rise to new, original and powerful methods of information processing. Starting from the exploration of the atom-photon interaction at the level of single particles, we see applications to the long-distance propagation of information thanks to a new type of quantum memory. This also opens up interesting prospects for quantum cryptography, which is theoretically unbreakable, unlike the classical encryption used today. Quantum information is a broader field of research than developed in this book. It has given rise to quantum computing, which is based on chains of logic gates created with qubits. There is much public excitement about the future of quantum computing in debate and about the “quantum supremacy” claimed by Google in autumn 2019, whose prototypes use superconducting qubits. However, with trapped and cooled ions such as those described in chapter 6, it is also possible to make qubits and build quantum logic gates, which operate with a lower error rate than the superconducting components of Google’s computer. This path is being pursued by many research teams, the challenge being to succeed in the scaling transition. Cold atoms in Rydberg states confined in optical tweezers, described in chapter 4, also seem to have a lot of potential for quantum computing and some pioneering start-ups have embarked on this adventure. Finally, ultra-cold electric dipolar molecules are also interesting candidates for the build-up of logic gates, as outlined in chapter 7, especially since they interact strongly at long distance.

Quantum simulation, a global approach to *N*-body physics

In the field of quantum simulation, there is no doubt that quantum gases hold great promise, with results expected for other areas of physics. As explained in detail in chapter 4, it is hoped that a quantum simulator built with cold atoms will lead to a better understanding of materials with strong quantum correlations. We have already mentioned atoms in Rydberg states, where the electrons are in orbits far away from the atomic nucleus. Organized in arbitrary arrays in optical tweezers, they are currently among the most studied systems in the cold atom community for applications in quantum simulation. Different families of particles, bosons or fermions, are used for simulations. In the case of bosons, simulation experiments based on Bose–Einstein condensates are developed in many directions, most of the time with theoretical models as support: on interacting spin chains, paramagnetic-antiferromagnetic phase transitions are simulated, with the formation of ferromagnetic domains; condensates coupled to the modes of two optical cavities can simulate the super-solid state; a condensate can experience a strong increase in the range of inter-particle interactions if it is immersed in a gas of ultra-cold fermions; arrays of small condensates are fascinating curiosities, etc. Many other studies focus on the non-equilibrium properties of Bose–Einstein condensates: shaking the sample generates spin waves; in quasi 1 D dimension far from equilibrium, a Bose gas can be interpreted by universal laws that can be generalized as far as cosmology. Ultra-cold fermionic quantum gases are also widely used to simulate the state of electrons in solids at room temperature. The possibility of arbitrarily varying the Feshbach resonance interactions, described in chapters 4 and 7, offers multiple possibilities. The so-called unitary maximum interaction regime can be reached, which opens up many perspectives for strongly interacting fermionic gases. Under such conditions, many studies have been carried out regarding their macroscopic properties, such as the thermodynamic ones. The future will be to probe these systems at the single atom scale, visualize pairs of fermions, break these pairs, and thus get as close as possible to the true nature of matter through simulation.

Matter waves like photons

The concept of quantum simulation is extended in chapter 5 with the description of Anderson localization experiments with ultra-cold atoms. Matter waves associated with atoms interfere; in the presence of disorder their expansion is blocked beyond a certain point. The analogy is strong with the lack of scattering of electromagnetic waves in a disordered medium, studied in condensed matter physics. The transposition to matter waves of phenomena studied with photons is a fascinating possibility offered by cold atoms. One example is the correlation experiments carried out at the Institut d'Optique with metastable helium condensates. With microchannel plates as detectors (see figure 8.3), situations analogous to the correlations between photons, exploited for a test of the Bell inequalities, can be achieved for massive

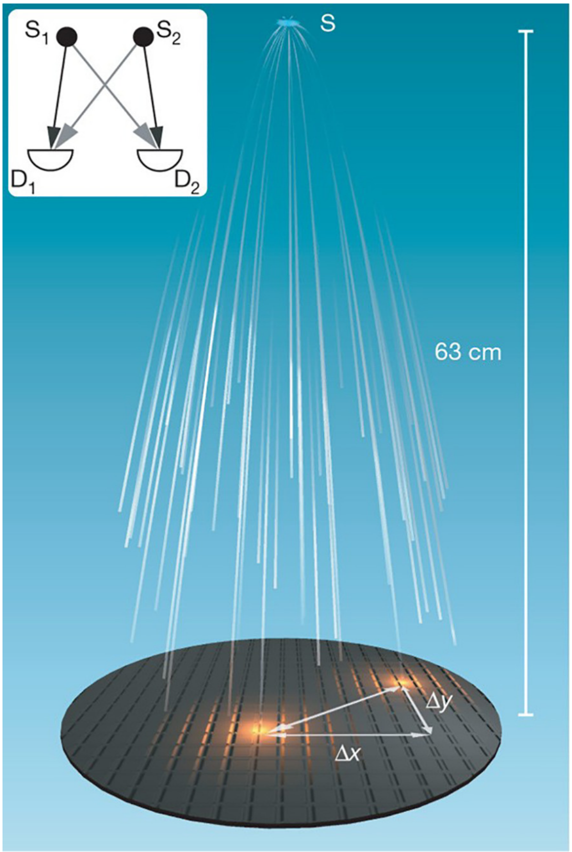

Fig. 8.3 – Condensed helium atoms in a metastable state of 20 eV internal energy are dropped into vacuum and fall onto a microchannel plate. On impact, their excitation energy releases electrons from the plate, allowing for time and space resolved detection of the atoms. This original detection method allows many studies of correlations between atoms and tests of quantum mechanics with matter waves.

particles – such as metastable helium atoms. The researchers want to answer the question: "Do the predictions of quantum mechanics work even for massive particles that are separated by a large distance?"

Chapter 5 reports on backscattering experiments with cold atoms which show a very striking analogy with the same phenomena observable with photons scattering in a material medium. It should be remembered that studies on collective behavior in the atom-light interaction were carried out by Robert Dicke in the 1950s, who, like Philip Anderson, an expert in interference effects, worked with him at Princeton. Robert Dicke's name is associated with collective effects when many atoms interact with a single mode of the electromagnetic field.

With cold atoms, these effects are currently at the heart of numerous theoretical and experimental studies, in particular the super-radiant laser effect, which allows coherence to be stored not in the empty space between two mirrors but in the coherences of atomic dipoles. This results in lasers emitting with extremely narrow linewidths. Sub-radiant modes, the dark counterpart of bright super-radiant states, are also studied with clouds of cold atoms, with potential for new quantum memories (see chapter 3).

Cold particles to test the fundamental laws of physics

This concluding chapter must finally mention all that cold atoms can bring to the knowledge of the fundamental laws of physics. We have encountered several occurrences of such opportunities throughout this book. Chapter 2 on metrology provides several examples. Tests of the invariance of fundamental constants, such as the fine structure constant α, can be based on the time shift of extremely accurate clocks making use of different cold atoms or ions. Comparing cold atom clocks on ground with those soon on board of the International Space Station will provide tests of general relativity of unparalleled accuracy, as discussed in chapter 2. Other fundamental tests are underway to verify the robustness of another fundamental principle of physics: the equivalence principle. According to this principle, the acceleration of an object subjected to a gravitational force is independent of its mass and chemical composition. The European Space Agency has considered a feasibility study for the STE-QUEST mission, the aim of which is to place two cold atom instruments in orbit: a clock and a differential interferometer. Other experiments are attempting to demonstrate differences in the fall of different atoms in order to answer the question: is Newton's equivalence principle (a feather falls as fast as an apple) still valid at the microscopic level? Researchers in Bremen and Hanover have built drop-towers several tens of meters high from which they release Bose–Einstein condensates in vacuum which can be regarded as "super-particles" (figure 8.4). The duration of the fall is sufficient to allow studying the expansion of the condensate in zero gravity. If the condensate is a mixture of rubidium and cesium, the question is whether the fall is identical for both species. For the time being, no difference is observed, but the accuracy of the test will increase with samples sent upwards in rockets. A Bose–Einstein condensate is already orbiting the Earth in the International Space Station and in the Chinese Spatial Space Station.

In another area, long-term progress for fundamental physics and cosmological speculation is expected with the knowledge of the antimatter properties.

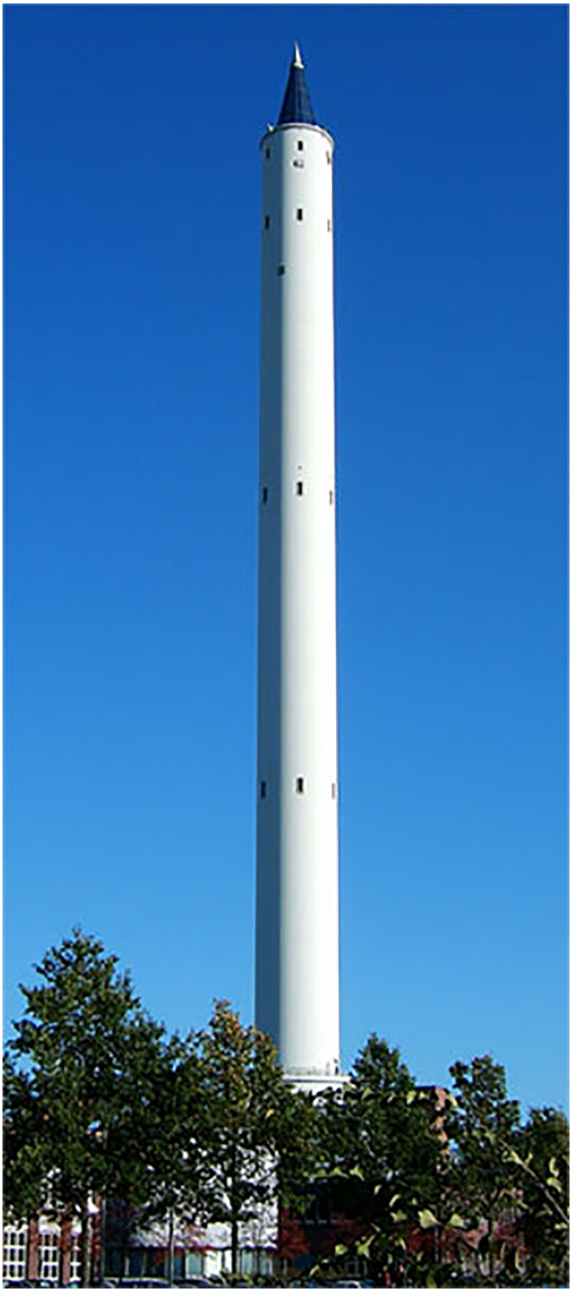

FIG. 8.4 – The 146 m high drop-tower at the University of Bremen in Germany, from the top of which physicists launch gas samples in the state of Bose Einstein condensate. The duration of the fall is of the order of 5 s, long enough to allow fundamental tests of the gravitation laws. Credit: CuttyP/CC BY-SA (http://creativecommons.org/licenses/by-sa/3.0/).

An important step is the fabrication of anti-hydrogen, for which cooled ion traps are an essential part of the devices under construction at CERN (see chapter 6).

Surprises abound, and there are more to come…

The ingenuity of cold atom researchers has also led to techniques for controlling collisions between atoms in their ground state, *i.e.* in the absence of laser excitation such as described in chapters 4 and 7. Control by Feshbach resonance cancels the outcome of collisions due to contact interactions, thus opening up the study of generally weaker interactions. This is the case for interactions between the magnetic dipoles of atoms which, unlike collisions between atoms, interact at greater distances. Novel and fascinating subjects appear, such as as recently observed quantum drops of matter, or super-solid states with frictionless transport properties. Cold atom researchers are not only able to switch interactions on and off (not possible if charged particles are involved, for example), but they can also control their sign and switch from attractive to repulsive interactions. As explained in chapter 4, such control also allows continuous switching of pairs of particles from a bosonic to a fermionic state, thus linking states of matter that have so far been studied separately. Several groups have proposed and are implementing experimental studies in which space dimensionality is an adjustable parameter. An example is the trapping of Bose–Einstein condensates in two dimensions, paving the way for new studies in low-dimensionality physics, an exciting topic for which the Nobel Prize was awarded to D. Thouless, F. D. Haldane and J. M. Kosterlitz in 2016 and the CNRS gold medal to Jean Dalibard in 2021. Condensate confinement with interacting neutral atomic fermions in one dimension has now been demonstrated, revealing specific physical phenomena in a case where very little has been attempted so far with interacting fermions, It is even possible to induce continuous transitions between dimensions or, by combining the internal states of atoms, to synthesize new dimensions. This makes it possible to investigate new topological effects with states more robust than others, such as knots that are difficult to untie.

This concluding chapter has not attempted to list all the new research directions in the field of cold atoms. It was meant to illustrate the activity of a creative community in which researchers, being open to both theoretical speculation and experiments, often have a specific advantage. It is also notable that the techniques and concepts developed in cold quantum gas physics are often adopted in other research fields. This was the case in the past with dipole traps, renamed optical tweezers, used daily in biology. Today, optical and evaporative cooling are frequent tools in condensed matter systems, for example in controlling thin membrane vibrations at the quantum level, or for polaritons condensation into the same collective quantum state. The extension of laser cooling to nano-spheres, already achieved in laboratories, and recently envisaged for cooling the very heavy mirrors of gravitational wave detectors, is another remarkable perspective. While the impact of cold atom research in cosmology is still very much in infancy, its capacity for perfect quantum control does provide means of exploring basic problems, such as the continuity between the microscopic and macroscopic world, an unsolved question since the birth of quantum mechanics. Predictions are difficult in a field that is in permanent renewal, constantly developing in new directions. We can bet that this will go on!

Index