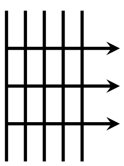
CY Cergy Paris Université **2019 – 2020**
Master 2 « Physique et Modélisation »
Parcours « Physique Théorique »

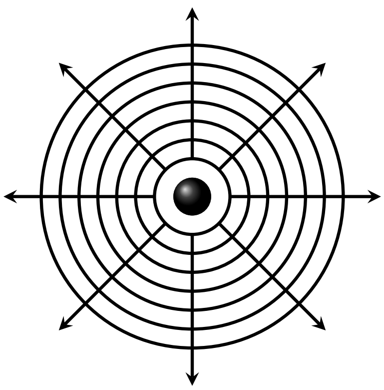
Tutorials of Advanced Quantum Mechanics

$$[\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')]_\pm = \delta_{\mathbf{k},\mathbf{k}'}$$

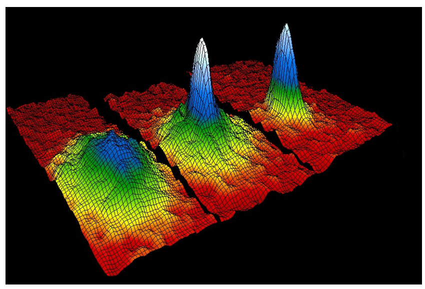
$$|\alpha\rangle = \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$



$\sim \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$



$\sim \dfrac{\mathrm{e}^{\mathrm{i}kr}}{r}$



Bose-Einstein condensation in a vapor of rubidium-87 atoms (JILA, 1995)

This document is available online at
http://lptms.u-psud.fr/pierre-elie_larre/enseignement_teaching/.

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Easy-to-Read References

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Tutorial I:
Identical Quantum Particles

Reminders

1 When are quantum particles said to be identical? Why are identical quantum particles in principle indistinguishable?

2 Show that the only possible states for a system of two identical quantum particles are symmetric or antisymmetric with respect to the exchange of the quantum numbers characterizing the particles. Infer the celebrated Pauli exclusion principle.

3 How do we call identical quantum particles forming a system with symmetric states? With antisymmetric states? Give examples of elementary particles, composite particles, and quasiparticles belonging to each family.

4 Recall the statement of the spin-statistics theorem.

Spin States for Identical Quantum Particles

5 How many independent symmetric, and then antisymmetric, spin states does a system of two identical quantum particles admit?

6 Particularize the results of Question **5** to the case where the particles are electrons. After expliciting it, label each of the independent symmetric and antisymmetric two-electron spin states in terms of its total spin and its projection.

7 Which natural degree of freedom must the electron spin be combined to so that your answers to Question **6** are not in contradiction with the Pauli exclusion principle?

Combined Position and Spin States for Identical Quantum Particles: Exchange Interaction in the Hydrogen Molecule

We model the hydrogen molecule as a system of two electrons with positions $\mathbf{r}_1$ and $\mathbf{r}_2$ in the electrostatic potentials of two fixed protons with positions $\mathbf{R}_1$ and $\mathbf{R}_2$. We denote by $\Psi_{\mathbf{R}_j}(\mathbf{r}_i)$ the ground-state position wavefunction of the electron $i \in \{1, 2\}$ in the electrostatic potential of the proton $j \in \{1, 2\}$ and introduce the overlap integral

$$\mathcal{S} = \int \Psi^*_{\mathbf{R}_1}(\mathbf{r})\, \Psi_{\mathbf{R}_2}(\mathbf{r})\, \mathrm{d}^3 r.$$

Of course, the two electrons, as well as the two protons, electrostatically interact with each other. Finally, we assume that it is energetically defavorable to find the two electrons in the vicinity of the same proton.

8 Why is the fixed-proton approximation licit? In this case, write down the Hamiltonian $\hat{H}$ of the hydrogen molecule.

9 What are the name, the expression, and the approximate value of the most probable distance between the proton and the electron of a hydrogen atom in its ground state? Reduce $\hat{H}$ to a simplified Hamiltonian $\hat{H}_0$ when the distance between the protons of the hydrogen molecule is much larger than this length scale. Find the wavefunction $\Psi_0(\mathbf{r}_1, \mathbf{r}_2)$ and the energy E_0 of the ground state of $\hat{H}_0$. You will not forget to account for the spin of the electrons and will denote by ε_0 the energy of a single hydrogen atom in its ground state.

10 We now come back to the complete Hamiltonian of Question **8**. Express the wavefunction $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ of its ground state in terms of appropriate combinations of position and spin wavefunctions. Then, after showing that

$$\begin{aligned}\int \Psi^*_{\mathbf{R}_j}(\mathbf{r}_1)\,\Psi^*_{\mathbf{R}_i}(\mathbf{r}_2)\;\hat{H}\;\Psi_{\mathbf{R}_\ell}(\mathbf{r}_1)\,\Psi_{\mathbf{R}_k}(\mathbf{r}_2)\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2 \\ = \int \Psi^*_{\mathbf{R}_i}(\mathbf{r}_1)\,\Psi^*_{\mathbf{R}_j}(\mathbf{r}_2)\;\hat{H}\;\Psi_{\mathbf{R}_k}(\mathbf{r}_1)\,\Psi_{\mathbf{R}_\ell}(\mathbf{r}_2)\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2\end{aligned}$$

for all $(i, j, k, \ell) \in \{1, 2\}^4$ such that $i \neq j$ and $k \neq \ell$, demonstrate that the associated energy

$$E = \int \Psi^*(\mathbf{r}_1, \mathbf{r}_2)\;\hat{H}\;\Psi(\mathbf{r}_1, \mathbf{r}_2)\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2$$

takes the form

$$\begin{aligned}E &= E_0 + \frac{\mathcal{C} \pm \mathcal{J}}{1 \pm |\mathcal{S}|^2}, \quad \text{where} \\ \mathcal{C} &= \int \Psi^*_{\mathbf{R}_1}(\mathbf{r}_1)\,\Psi^*_{\mathbf{R}_2}(\mathbf{r}_2)\,(\hat{H} - \hat{H}_0)\,\Psi_{\mathbf{R}_1}(\mathbf{r}_1)\,\Psi_{\mathbf{R}_2}(\mathbf{r}_2)\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2 \quad \text{and} \\ \mathcal{J} &= \int \Psi^*_{\mathbf{R}_1}(\mathbf{r}_1)\,\Psi^*_{\mathbf{R}_2}(\mathbf{r}_2)\,(\hat{H} - \hat{H}_0)\,\Psi_{\mathbf{R}_2}(\mathbf{r}_1)\,\Psi_{\mathbf{R}_1}(\mathbf{r}_2)\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2.\end{aligned}$$

The integrals $\mathcal{C}$ and $\mathcal{J}$ are respectively called the Coulomb integral and the exchange integral.

11 We denote by $\hat{\mathbf{S}}_i$ the spin operator associated to the electron $i \in \{1, 2\}$. What are the eigenvalues of $(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)^2$ and $\hat{\mathbf{S}}_i{}^2$? Infer the ones of $\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2$ and deduce that the ground state of $\hat{H}$ is also an eigenstate of the Heisenberg Hamiltonian

$$\hat{H}_\mathrm{H} = E_0 - J\,\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2, \quad \text{where} \quad J = \frac{2}{\hbar^2}\,\frac{\mathcal{J} - \mathcal{C}\,|\mathcal{S}|^2}{1 - |\mathcal{S}|^4}.$$

Comment the expression of $\hat{H}_\mathrm{H}$ given above.

12 Establish a simple expression for the exchange constant J in the asymptotic limit of Question **9**, assuming here that $\hat{H} - \hat{H}_0$, although small in this limit, is nonzero. In this case, what sign must the exchange integral $\mathcal{J}$ have in order for the coupling between $\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$ to be ferromagnetic? Antiferromagnetic?

Tutorial II: Quantum Harmonic Oscillator

Reminders

We consider a one-dimensional quantum harmonic oscillator[1] of mass m and angular frequency ω.

1 Recall the commutation relation between the position operator $\hat{x}$ and the momentum operator $\hat{p}$ of the system. Express its Hamiltonian $\hat{H}$ in terms of $\hat{x}$ and $\hat{p}$. Verify that $\hbar\,\omega$,

$$x_0 = \sqrt{\frac{\hbar}{m\,\omega}}, \quad \text{and} \quad p_0 = \sqrt{\hbar\,m\,\omega}$$

are respectively the typical energy, position, and momentum scales of the problem.

2 We now introduce the dimensionless operator

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + \mathrm{i}\,\frac{\hat{p}}{p_0}\right).$$

Is $\hat{a}$ Hermitian? Establish the commutation relation between $\hat{a}$ and its Hermitian conjugate $\hat{a}^\dagger$. Express $\hat{H}$ in terms of the operator

$$\hat{n} = \hat{a}^\dagger\,\hat{a}.$$

Infer that $\hat{H}$ and $\hat{n}$ share the same eigenstates.

3 We denote by $|n\rangle$ a unit eigenstate of $\hat{n}$ with the eigenvalue n. Show that $n \geqslant 0$. Then, demonstrate that

$$\hat{a}\,|0\rangle = 0 \quad \text{and that for } n > 0, \quad \hat{n}\,\hat{a}^k\,|n\rangle = (n-k)\,\hat{a}^k\,|n\rangle$$

for all $k \in [\![1, k_n]\!]$, where k_n is to determine as a function of n. Infer that $n \in \mathbb{N}$. What does

$$\mathcal{E} = \left\{\hbar\,\omega\left(n + \frac{1}{2}\right),\, n \in \mathbb{N}\right\}$$

correspond to?

4 Demonstrate that for all $n \in \mathbb{N}$,

$$\hat{a}\,|n+1\rangle = \sqrt{n+1}\,|n\rangle \quad \text{and} \quad \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle.$$

Justify the namings "annihilation operator," "creation operator," and "number operator" for $\hat{a}$, $\hat{a}^\dagger$, and $\hat{n}$, respectively. From the second of the preceding identities, infer that any eigenstate $|n\rangle$ of $\hat{H}$ can be expressed in terms of the ground state $|0\rangle$ as

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|0\rangle.$$

[1] Henceforth denoted by "QHO" in the following.

5 Find the ground-state wavefunction $\psi_0(x)$ of the system and show that the wavefunction $\psi_n(x)$ of its nth eigenstate relates to $\psi_0(x)$ as

$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \left(\frac{x}{x_0} - x_0 \frac{\mathrm{d}}{\mathrm{d}x} \right)^n \psi_0(x).$$

6 The potential $V(x)$ in which the quantum particle of mass m evolves is often not harmonic. Nevertheless, it frequently presents at least one minimum. We denote by x_* the position of this minimum. Taylor expand $V(x)$ around $x = x_*$ up to the second order. Why does the QHO model constitute a building block in quantum mechanics?

7 What is the energy spectrum of a quantum particle of mass m trapped in a harmonic potential of the form

$$V(\{x_i\}_{i=1}^{d}) = \frac{m}{2} \sum_{i=1}^{d} {\omega_i}^2\, {x_i}^2 ?$$

The Cartesian-coordinate set $\{x_i\}_{i=1}^{d}$ specifies the position of the particle in dimension $d \geqslant 2$ and the angular frequencies of the set $\{\omega_i\}_{i=1}^{d}$ are all different, which breaks isotropy.

8 Recall the expression of the Hamiltonian of a gas of noninteracting identical quantum particles (bosons or fermions) in the second-quantization language. Conclude, again, on the importance of the QHO model in quantum mechanics.

Statistical Physics of the QHO: The Black-Body Spectrum

We consider a cubic cavity of size L containing atoms and photons in thermal equilibrium at the temperature T. The number of atoms is N and each of them is simply modeled as a two-level system whose excited state $|\mathrm{e}\rangle$ is separated from the ground state $|\mathrm{g}\rangle$ by the energy $\hbar\omega$. From Questions **9** to **12**, we search for the expression of n, the average number of photons with angular frequency ω, in two different ways. Then, from Questions **13** to **16**, we search for the one of $\mathrm{d}E/\mathrm{d}\omega$, the energy spectral density of electromagnetic modes in the cavity, and discuss the celebrated ultraviolet-catastrophe prediction of late 19th century/early 20th century.

9 Express the ratio of N_e, the number of atoms in the excited state, to N_g, the number of atoms in the ground state, as a function of $\hbar\omega$ and $k_\mathrm{B}T$, where k_B is the Boltzmann constant.

10 What is the photon absorption rate due to atoms in the ground state, $\Gamma_\uparrow$? Same question for $\Gamma_\downarrow$, the photon emission rate due to atoms in the excited state. You will not forget to account for spontaneous emission.

11 In thermal equilibrium, the upward and downward transition rates must balance. Deduce an expression for n. How is this statistical distribution called? What is its behavior when $\hbar\omega \ll k_\mathrm{B}T$? What does this limit correspond to?

12 Assuming that the gas of photons with angular frequency ω behaves as a collection of QHOs, express its Hamiltonian $\hat{H}$ as a function of $\hbar\omega$ and $\hat{n}$, the operator counting the photons with angular frequency ω. Then, find again the expression of n as the expectation value of $\hat{n}$ in the canonical ensemble:

$$n = \langle \hat{n} \rangle = \frac{\mathrm{tr}\{\hat{n} \exp[-\hat{H}/(k_\mathrm{B}T)]\}}{\mathrm{tr}\{\exp[-\hat{H}/(k_\mathrm{B}T)]\}}.$$

13 The position wavefunction of a photon in the cavity consists in a plane wave with wavevector $\mathbf{k}$:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}}.$$

Assuming that the cavity is provided with the periodic boundary conditions, show that $\mathbf{k}$ is quantized (the origin of the coordinates coincides with the center of the box). How many electromagnetic modes does some domain of volume d^3k in wavevector space contain? Do not forget that each photon admits two independent polarization states.

14 Despite the presence of atoms, we assume that the dispersion relation $\omega(k)$ of the photons in the cavity is the one they have in vacuum. Recall it. How many electromagnetic modes does some angular-frequency interval of length $\mathrm{d}\omega$ contain?

15 Combine the preceding result with the expression for n established in Questions **11** and **12** to obtain the energy $\mathrm{d}E$ of the electromagnetic modes lying in some angular-frequency interval of length $\mathrm{d}\omega$. What is the name of the energy spectral density $\mathrm{d}E/\mathrm{d}\omega$ you just found? Of its classical approximation $(\mathrm{d}E/\mathrm{d}\omega)_{\mathrm{class}}$?

16 Plot on a same graph $\mathrm{d}E/\mathrm{d}\omega$ and $(\mathrm{d}E/\mathrm{d}\omega)_{\mathrm{class}}$ as a function of $\hbar\,\omega/(k_{\mathrm{B}}\,T)$. Comment.

Entertainment

We consider a gas of free identical fermions (bosons) of mass m and spin s in a cubic box of size L provided with the periodic boundary conditions and in thermal and chemical equilibrium with an external reservoir of energy and particles. We respectively denote by T and μ the temperature and the chemical potential of the gas. Show that the anticommutation (commutation) relations verified by the ladder operators of the fermionic (bosonic) system lead to

$$\langle \hat{n}_{\mathbf{k}} \rangle_{\binom{\mathrm{F}}{\mathrm{B}}} = \frac{2\,s+1}{\exp[(E_{\mathbf{k}}-\mu)/(k_{\mathrm{B}}\,T)]\,\binom{+}{-}\,1}$$

for the average number of fermions (bosons) in the quantum state with wavevector $\mathbf{k}$, where the energy $E_{\mathbf{k}} = \hbar^2\,\mathbf{k}^2/(2\,m)$ and k_{B} is the Boltzmann constant.

Tutorial III: QHO Coherent States

In this tutorial, we consider a one-dimensional QHO of mass m and angular frequency ω. In Tutorial **II**, you showed that its Hamiltonian

$$\hat{H} = \frac{m\,\omega^2}{2}\,\hat{x}^2 + \frac{1}{2\,m}\,\hat{p}^2$$

can be expressed in terms of the annihilation operator

$$\hat{a} = \sqrt{\frac{m\,\omega}{2\,\hbar}}\,\hat{x} + \mathrm{i}\,\sqrt{\frac{1}{2\,\hbar\,m\,\omega}}\,\hat{p}$$

and the creation operator $\hat{a}^\dagger$ as

$$\hat{H} = \hbar\,\omega\left(\hat{a}^\dagger\,\hat{a} + \frac{1}{2}\right),$$

the eigenstates $|n\rangle$ and the corresponding eigenvalues $\hbar\,\omega\,(n+1/2)$ of which are labeled by $n \in \mathbb{N}$. The oscillator states $|n\rangle$ are usually called “number states” or “Fock states.” Our goal here is to study another family of oscillator states called “coherent states.”

Definition and Properties

Restricting to the case of the one-dimensional QHO considered above, a coherent state $|\alpha\rangle$ is mathematically defined to be the (unique) eigenstate of the annihilation operator associated to the eigenvalue α:

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle.$$

1 Is $\hat{a}$ Hermitian? Infer the set in which the domain of definition of its spectrum is included.

2 How does a coherent state $|\alpha\rangle$ decompose on the (orthonormal) number-state basis $\{|n\rangle,\, n \in \mathbb{N}\}$? You will ensure that $|\alpha\rangle$ is normalized to unity.

3 Show that the number of particles in a coherent state $|\alpha\rangle$ is distributed according to a Poisson law, the parameter of which you will determine. How do its mean value and its variance relate to the latter? Give examples of physical systems characterized by a Poisson distribution.

4 Explicitly show that two different coherent states $|\alpha\rangle$ and $|\beta\rangle$ are not orthogonal. Is it in accordance with your answer to Question **1**? Under which constraint on the complex numbers α and β do $|\alpha\rangle$ and $|\beta\rangle$ become orthogonal?

5 Establish that the coherent states satisfy the closure relation

$$\int |\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha = 1,$$

where $\mathrm{d}^2\alpha$ is a shorthand notation for $\mathrm{dRe}(\alpha)\,\mathrm{dIm}(\alpha)/\pi$.

6 How does a number state $|n\rangle$ decompose on the coherent-state set $\{|\alpha\rangle,\, \alpha \in \mathbb{C}\}$? Is such a decomposition unique?

7 At the time $t = 0$, we prepare the system in the coherent state

$$|\psi_\alpha(0)\rangle = |\alpha\rangle.$$

What is the state $|\psi_\alpha(t)\rangle$ of the system at a time $t > 0$? Is this state coherent?

8 Calculate the mean values $x_\alpha(t)$ and $p_\alpha(t)$ and the standard deviations $\Delta x_\alpha(t)$ and $\Delta p_\alpha(t)$ of the position and momentum operators $\hat{x}$ and $\hat{p}$ in the state $|\psi_\alpha(t)\rangle$ of Question **7**. After representing $\alpha \neq 0$ in polar coordinates, place the point $(x_\alpha(t), p_\alpha(t))$ and its uncertainty bars $\Delta x_\alpha(t)$ and $\Delta p_\alpha(t)$ on a diagram representing the phase space, first for $t = 0$ and then for $t > 0$.

9 Calculate the product $\Delta x_\alpha(t)\, \Delta p_\alpha(t)$ and infer the shape of $|\psi_\alpha(t)\rangle$ in the position or momentum representation.

10 What do $\Delta x_\alpha(t)/x_\alpha(t)$ and $\Delta p_\alpha(t)/p_\alpha(t)$ tend to when $|\alpha| \to \infty$? What does it mean?

Alternative Definition

For any complex number α, we define the operator

$$\hat{D}(\alpha) = \exp(\alpha\, \hat{a}^\dagger - \alpha^*\, \hat{a}).$$

We also recall that the identity

$$\exp(\hat{A} + \hat{B}) = \exp(\hat{A})\exp(\hat{B})\exp(-[\hat{A}, \hat{B}]/2)$$

holds if the operators $\hat{A}$ and $\hat{B}$ commute with their commutator.

11 What is $\hat{D}(0)$ equal to? For any complex numbers α and β, show that

$$\hat{D}(\alpha)^\dagger = \hat{D}(-\alpha),$$

that $\hat{D}(\alpha)$ is unitary, and that

$$\hat{D}(\alpha)\, \hat{D}(\beta) = \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(\alpha^*\beta)}\, \hat{D}(\alpha + \beta).$$

12 Demonstrate that any coherent state $|\alpha\rangle$ may be deduced from the vacuum state $|0\rangle$ through

$$|\alpha\rangle = \hat{D}(\alpha)\, |0\rangle,$$

which may be used as a definition for $|\alpha\rangle$.

13 For any complex number α, justify the naming "displacement operator" for $\hat{D}(\alpha)$ by demonstrating that the effect of applying $\hat{D}(\alpha)$ in a similarity transformation of $\hat{a}$ results in the displacement of the latter with a magnitude $\pm\,\alpha$, that is,

$$\hat{D}(\alpha)^{-1}\, \hat{a}\, \hat{D}(\alpha) = \hat{a} + \alpha \quad \text{and} \quad \hat{D}(\alpha)\, \hat{a}\, \hat{D}(\alpha)^{-1} = \hat{a} - \alpha.$$

Quantum Mechanics in the Interaction Picture

We consider a quantum system whose dynamics in the Schrödinger picture is ruled by the Hamiltonian $\hat{H}_0 + \hat{H}_1(t)$, where $\hat{H}_0$ is independent of time and well understood and $\hat{H}_1(t)$ describes some harder-to-analyze perturbation to the system. By definition, the operators $\hat{O}_\mathrm{I}(t)$ and the states $|\psi_\mathrm{I}(t)\rangle$ in the interaction picture relate to the operators $\hat{O}$ and the states $|\psi(t)\rangle$ in the Schrödinger picture as

$$\hat{O}_\mathrm{I}(t) = \exp(\mathrm{i}\,\hat{H}_0\,t/\hbar)\,\hat{O}\exp(-\mathrm{i}\,\hat{H}_0\,t/\hbar) \quad \text{and} \quad |\psi_\mathrm{I}(t)\rangle = \exp(\mathrm{i}\,\hat{H}_0\,t/\hbar)\,|\psi(t)\rangle.$$

14 Write down the time-evolution equations of $\hat{O}_\mathrm{I}(t)$ and $|\psi_\mathrm{I}(t)\rangle$. Why is the interaction picture useful?

15 Verify that the expectation-value operation is independent of the picture considered (interaction or Schrödinger), that is,

$$\langle\psi_\mathrm{I}(t)|\,\hat{O}_\mathrm{I}(t)\,|\psi_\mathrm{I}(t)\rangle = \langle\psi(t)|\,\hat{O}\,|\psi(t)\rangle.$$

Trapped Ion Coupled to an Optical Field

An ion of mass m and charge q moves along the x axis in a harmonic potential of angular frequency ω. It is furthermore immersed in a classical electric field of the form

$$\mathbf{E}(t) = E_0 \sin(\omega\,t - \phi)\,\mathbf{e}_x \quad (E_0 \in \mathbb{R}).$$

Treated in a quantum mechanical way, the electric dipole moment

$$\hat{\mathbf{p}} = q\,\hat{x}\,\mathbf{e}_x$$

of the ion couples to $\mathbf{E}(t)$ through the interaction Hamiltonian

$$\hat{H}_1(t) = -\hat{\mathbf{p}}\cdot\mathbf{E}(t).$$

16 Express the free Hamiltonian $\hat{H}_0$ and the interaction Hamiltonian in the interaction picture $(\hat{H}_1)_\mathrm{I}(t)$ in terms of the annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$ of the ion.

17 Show that $(\hat{H}_1)_\mathrm{I}(t)$ becomes time-independent in the secular approximation.

18 At the time $t = 0$, we assume that the ion is in the vacuum state:

$$|\psi_\mathrm{I}(0)\rangle = |0\rangle.$$

In the secular approximation considered in the preceding question, demonstrate that the ion must be in the coherent state

$$|\psi_\mathrm{I}(t)\rangle = \left|-\frac{q\,E_0\,\mathrm{e}^{\mathrm{i}\phi}}{2\sqrt{2\,\hbar\,m\,\omega}}\,t\right\rangle$$

a while later.

Tutorial IV:
Low-Energy Quantum Scattering

Reminders

A quantum particle of mass m, energy E, and wavenumber

$$k = |\mathbf{k}| = \frac{\sqrt{2\,m\,E}}{\hbar}$$

scatters off a time-independent central potential $V(r = |\mathbf{r}|)$ of scattering length a. Its wavefunction $\Psi(\mathbf{r})$ is solution of the stationary Schrödinger equation

$$E\,\Psi = -\frac{\hbar^2}{2\,m}\,\Delta\Psi + V(r)\,\Psi = -\frac{\hbar^2}{2\,m}\left[\frac{1}{r}\,\frac{\partial^2}{\partial r^2}(r\,\Psi) + \frac{1}{r^2}\,\Delta_{\mathbb{S}^2}\Psi\right] + V(r)\,\Psi,$$

where $\Delta_{\mathbb{S}^2}$ denotes the Laplacian on the unit 2-sphere $\mathbb{S}^2$.

1 The length a characterizes the scattering of the particle in the low-energy limit. Express the latter in terms of k and a. What does $V(r)$ tend to in the large-distance limit $r \gg |a|$?

2 In the low-energy limit, show that

$$\psi(r) = r \int_{\mathbb{S}^2} \Psi(\mathbf{r})\,\mathrm{d}^2\Omega$$

satisfy the following identities:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2} = \frac{2\,m}{\hbar^2}\,V(r)\,\psi, \quad \psi(r = 0) = 0, \quad \text{and} \quad \psi(r \gg |a|) \simeq A\,r + B,$$

where A and B are two arbitrary constants.

3 In the low-energy and large-distance limits, we recall that $\Psi(\mathbf{r})$ may be cast (up to some normalization factor) in the form

$$\Psi(\mathbf{r}) \simeq \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} + f(k)\,\frac{\mathrm{e}^{\mathrm{i}kr}}{r}.$$

Provide a physical interpretation of this expansion. What is the name of $f(k)$? How does it relate to a? Infer that

$$\psi(r \gg |a|) \simeq C\,(r - a),$$

where C is a constant.

4 What is the condition satisfied by the maximum of $V(r)$, m, and a for the low-energy Born approximation to be applicable? What is the expression of a in this limit?

Hard-Sphere Potential

In this problem, the potential introduced in the preceding section reads

$$V(r) = \begin{cases} V_0 \geqslant 0 & \text{if} \quad r \leqslant R \\ 0 & \text{if} \quad r > R \end{cases}.$$

5 Determine the scattering length a as a function of V_0 and R. What is its sign? Show that one recovers the result predicted by the Born theory when $V_0 \to 0$.

6 What happens to a when $V_0 \to \infty$, R being kept constant? In this case, $V(r)$ is said to be of hard sphere.

7 What happens to a when $V_0 \to \infty$ and $R \to 0$,

$$\int V(r)\, \mathrm{d}^3 r = \frac{4\,\pi\, V_0\, R^3}{3}$$

being kept constant? In this case,

$$V(r) = \frac{4\,\pi\, V_0\, R^3}{3}\, \delta^{(3)}(\mathbf{r}),$$

where $\delta^{(3)}$ is the three-dimensional Dirac "function."

Square-Well Potential

We consider the same problem as before except that we now assume that $V_0 \leqslant 0$. In this case, $V(r)$ is a square-well-shaped function of r.

8 Show that the scattering length a displays discrete resonances as one decreases the value of V_0, R being kept constant. Relate the position of these resonances to the number of bound states in the potential $V(r)$.

9 Recover the result predicted by the Born theory when $V_0 \to 0$. What is the sign of a in this case?

Tutorial V:
Imperfect Bose Gas

An ultracold quantum gas of N interacting bosonic atoms of mass m with no apparent internal degrees of freedom is contained in a large cubic cavity of size L provided with the periodic boundary conditions (the origin of the coordinates coincides with the center of the box). The "first-quantization" Hamiltonian of the quantum many-body system is expressed as a function of the position and momentum operators $\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2, \ldots, \hat{\mathbf{r}}_N$ and $\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2, \ldots, \hat{\mathbf{p}}_N$ of the atoms as

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i{}^2}{2\,m} + \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} V(|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|),$$

where $V(|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|)$ describes the interaction between the atoms i and $j \neq i$.

Preliminaries

1 We generically denote by $\{\psi_\lambda(\mathbf{r})\}_\lambda$ the orthonormal and complete set (assumed to be discrete for the sake of simplicity) of the single-particle wavefunctions. The operator destroying an atom at the point $\mathbf{r}$ may be expanded as

$$\hat{\Psi}(\mathbf{r}) = \sum_\lambda \psi_\lambda(\mathbf{r})\, \hat{a}(\lambda),$$

where $\hat{a}(\lambda)$ is the annihilation operator in the single-particle quantum state of wavefunction $\psi_\lambda(\mathbf{r})$. Verify that

$$[\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')] = \delta^{(3)}(\mathbf{r} - \mathbf{r}') \quad \text{and} \quad [\hat{\Psi}(\mathbf{r}), \hat{\Psi}(\mathbf{r}')] = 0,$$

where the Hermitian conjugate of $\hat{\Psi}(\mathbf{r})$, $\hat{\Psi}^\dagger(\mathbf{r})$, creates an atom at the point $\mathbf{r}$, and $\delta^{(3)}$ is the three-dimensional Dirac "function."

2 Establish that the "second-quantization" Hamiltonian $\hat{H}$ and the atom-number operator $\hat{N}$ of the quantum many-body system respectively read

$$\hat{H} = -\frac{\hbar^2}{2\,m} \int \hat{\Psi}^\dagger(\mathbf{r})\, \Delta \hat{\Psi}(\mathbf{r})\, \mathrm{d}^3 r + \frac{1}{2} \int \hat{\Psi}^\dagger(\mathbf{r})\, \hat{\Psi}^\dagger(\mathbf{r}')\, V(|\mathbf{r} - \mathbf{r}'|)\, \hat{\Psi}(\mathbf{r}')\, \hat{\Psi}(\mathbf{r})\, \mathrm{d}^3 r\, \mathrm{d}^3 r' \quad \text{and}$$

$$\hat{N} = \int \hat{\Psi}^\dagger(\mathbf{r})\, \hat{\Psi}(\mathbf{r})\, \mathrm{d}^3 r.$$

Reexpress the kinetic term in $\hat{H}$ in the light of the identity

$$\int f_1(\mathbf{r})\, \Delta f_2(\mathbf{r})\, \mathrm{d}^3 r = -\int \nabla f_1(\mathbf{r}) \cdot \nabla f_2(\mathbf{r})\, \mathrm{d}^3 r,$$

which you will indicate the condition of validity. In the following, we will deal with the grand-canonical version of $\hat{H}$,

$$\hat{K} = \hat{H} - \mu\, \hat{N},$$

where μ is the chemical potential of the gas.

3 The gas is assumed to be dilute. In this case, justify that $V(|\mathbf{r}-\mathbf{r}'|)$ can be approximated by a contact potential:

$$V(|\mathbf{r}-\mathbf{r}'|) \simeq g\,\delta^{(3)}(\mathbf{r}-\mathbf{r}'),$$

where g is a parameter describing the atom-atom interactions which we will not derive the expression. Accordingly simplify the expression of $\hat{K}$ defined in Question 2. We finally suppose that the atoms repulsively interact with each other. What is the sign of g in this case?

4 The gas is assumed to be homogeneous. In this case, justify that the single-particle wavefunctions are plane waves with discretized wavevectors:

$$\psi_\lambda(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r}) = \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}} \quad \text{with} \quad \mathbf{k} \in \frac{2\pi}{L}\,\mathbb{Z}^3.$$

Demonstrate that this implies the useful approximations

$$\sum_{\mathbf{k}} f(\mathbf{k}) \simeq \left(\frac{L}{2\pi}\right)^3 \int f(\mathbf{k})\,\mathrm{d}^3k \quad \text{and} \quad \delta_{\mathbf{k},\mathbf{k}'} \simeq \left(\frac{2\pi}{L}\right)^3 \delta^{(3)}(\mathbf{k}-\mathbf{k}').$$

Bogoliubov Hamiltonian

As bosons, the atoms of the gas tend to accumulate in the quantum state with wavevector $\mathbf{k}=0$ as their temperature T is lowered down to some critical value T_c. Provided they weakly interact, which we assume from now on, the occupancy N_0 of the $\mathbf{k}=0$ state becomes of the order of N at very low temperature, leaving the $\mathbf{k}\neq 0$ states weakly populated:

$$\delta N = N - N_0 \ll N \quad \text{as} \quad T \ll T_\mathrm{c}.$$

This spectacular quantum phenomenon, known as Bose-Einstein condensation, was predicted in the case of noninteracting bosons by Einstein in 1925 and was first observed in an ultracold vapor of rubidium-87 atoms by the group of Cornell and Wieman in 1995.

5 As implicitly stated in the introduction of the tutorial, T is here supposed to be much lower than T_c. Demonstrate that this makes it possible to split $\hat{\Psi}(\mathbf{r})$ in the form

$$\hat{\Psi}(\mathbf{r}) = \sqrt{n_0} + \delta\hat{\Psi}(\mathbf{r}),$$

where the c-number[2] $\sqrt{n_0}$ involves the density of the condensate,

$$n_0 = \frac{N_0}{L^3}, \quad \text{and where} \quad \delta\hat{\Psi}(\mathbf{r}) = \frac{1}{L^{3/2}} \sum_{\mathbf{k}\neq 0} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\,\hat{a}(\mathbf{k})$$

is a small quantum correction to $\sqrt{n_0}$.

[2] This is an old nomenclature used by Dirac, which refers to "classical," commuting quantities, in opposition to the terminology "q-number," which refers to "quantum," noncommuting quantities.

6 Using the previous splitting of $\hat{\Psi}(\mathbf{r})$, expand the grand-canonical Hamiltonian $\hat{K}$ of Question **3** in powers of $\delta\hat{\Psi}(\mathbf{r})$ and $\delta\hat{\Psi}^\dagger(\mathbf{r})$, retaining only the linear and quadratic terms, and cast it in the form

$$\begin{aligned}
\hat{K} &= K_0 + \hat{K}_1 + \hat{K}_2 + \cdots, \quad \text{where} \\
K_0 &= \left(\frac{g n_0}{2} - \mu\right) N_0, \\
\hat{K}_1 &= (g n_0 - \mu)\sqrt{n_0} \int [\delta\hat{\Psi}(\mathbf{r}) + \delta\hat{\Psi}^\dagger(\mathbf{r})]\, \mathrm{d}^3 r, \\
\hat{K}_2 &= \int \left\{ \frac{\hbar^2}{2\,m} \nabla\delta\hat{\Psi}^\dagger(\mathbf{r}) \cdot \nabla\delta\hat{\Psi}(\mathbf{r}) + (2\,g n_0 - \mu)\, \delta\hat{\Psi}^\dagger(\mathbf{r})\, \delta\hat{\Psi}(\mathbf{r}) + \frac{g n_0}{2} [\delta\hat{\Psi}^2(\mathbf{r}) + (\delta\hat{\Psi}^\dagger)^2(\mathbf{r})] \right\} \mathrm{d}^3 r,
\end{aligned}$$

and "$\cdots$" refers to the terms we chose to neglect.

7 Infer that the "condensate wavefunction" $\sqrt{n_0}$ extremizes $\hat{K}$ if, and only if,

$$\mu = g n_0,$$

which we consider from now on. Our quantum many-body system is then described by the following effective quadratic grand-canonical Hamiltonian:

$$\begin{aligned}
\hat{K}_\mathrm{B} &= K_0 + \hat{K}_2 \\
&= -\frac{g n_0}{2} N_0 + \int \left\{ \frac{\hbar^2}{2\,m} \nabla\delta\hat{\Psi}^\dagger(\mathbf{r}) \cdot \nabla\delta\hat{\Psi}(\mathbf{r}) + g n_0\, \delta\hat{\Psi}^\dagger(\mathbf{r})\, \delta\hat{\Psi}(\mathbf{r}) + \frac{g n_0}{2} [\delta\hat{\Psi}^2(\mathbf{r}) + (\delta\hat{\Psi}^\dagger)^2(\mathbf{r})] \right\} \mathrm{d}^3 r,
\end{aligned}$$

known as the Bogoliubov Hamiltonian.

Bogoliubov Spectrum

At this stage, $\hat{K}_\mathrm{B}$ is not diagonal in the operators $\delta\hat{\Psi}(\mathbf{r})$ and $\delta\hat{\Psi}^\dagger(\mathbf{r})$ [or $\hat{a}(\mathbf{k})$ and $\hat{a}^\dagger(\mathbf{k})$].[3] To diagonalize it, we introduce the so-called Bogoliubov transformation

$$\hat{a}(\mathbf{k} \neq 0) \longmapsto \hat{b}(\mathbf{k}) = u(k)\, \hat{a}(\mathbf{k}) - v(k)\, \hat{a}^\dagger(-\mathbf{k}),$$

where u and v are real functions of $k = |\mathbf{k}|$.

8 Which constraint do the so-called Bogoliubov amplitudes $u(k)$ and $v(k)$ have to satisfy in order for the Bogoliubov transformation to be canonical, that is, such that

$$[\hat{b}(\mathbf{k}), \hat{b}^\dagger(\mathbf{k}')] = [\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')] = \delta_{\mathbf{k},\mathbf{k}'} \quad \text{and} \quad [\hat{b}(\mathbf{k}), \hat{b}(\mathbf{k}')] = [\hat{a}(\mathbf{k}), \hat{a}(\mathbf{k}')] = 0?$$

Infer that there exists a hyperbolic angle $\theta(k)$ such that

$$u(k) = \cosh\theta(k) \quad \text{and} \quad v(k) = \sinh\theta(k).$$

[3] That is, not of the form $\int \delta\hat{\Psi}^\dagger(\mathbf{r})\, (\text{Something})\, \delta\hat{\Psi}(\mathbf{r})\, \mathrm{d}^3 r$ [or $\sum_{\mathbf{k}\neq 0} \hat{a}^\dagger(\mathbf{k})\, (\text{Something})\, \hat{a}(\mathbf{k})$].

9 Express $\delta\hat{\Psi}(\mathbf{r})$ in the form

$$\delta\hat{\Psi}(\mathbf{r}) = \frac{1}{L^{3/2}} \sum_{\mathbf{k}\neq 0} [u(k)\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\,\hat{b}(\mathbf{k}) + v(k)\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\,\hat{b}^\dagger(\mathbf{k})]$$

and show that

$$\begin{aligned}\hat{K}_{\mathrm{B}} = E_0 + \sum_{\mathbf{k}\neq 0} \Bigg\{ \Bigg[\left(\frac{\hbar^2\,k^2}{2\,m} + g n_0\right) (u^2(k) + v^2(k)) + 2\,g n_0\,u(k)\,v(k) \Bigg] \hat{b}^\dagger(\mathbf{k})\,\hat{b}(\mathbf{k}) \\ + \Bigg[\left(\frac{\hbar^2\,k^2}{2\,m} + g n_0\right) u(k)\,v(k) + \frac{g n_0}{2}\,(u^2(k) + v^2(k)) \Bigg] [\hat{b}(\mathbf{k})\,\hat{b}(-\mathbf{k}) + \hat{b}^\dagger(\mathbf{k})\,\hat{b}^\dagger(-\mathbf{k})] \Bigg\}, \quad \text{where} \\ E_0 = -\frac{g n_0}{2}\,N_0 + \sum_{\mathbf{k}\neq 0} \Bigg[\left(\frac{\hbar^2\,k^2}{2\,m} + g n_0\right) v^2(k) + g n_0\,u(k)\,v(k) \Bigg].\end{aligned}$$

10 We force $\hat{K}_{\mathrm{B}}$ to become diagonal in the operators $\hat{b}(\mathbf{k})$ and $\hat{b}^\dagger(\mathbf{k})$ by canceling out the coefficient weighting the nondiagonal operator $\hat{b}(\mathbf{k})\,\hat{b}(-\mathbf{k}) + \hat{b}^\dagger(\mathbf{k})\,\hat{b}^\dagger(-\mathbf{k})$. Infer that

$$\theta(k) = \frac{1}{2} \ln\left[\frac{E_{\mathrm{B}}(k)}{\hbar^2\,k^2/(2\,m)}\right],$$

where we introduced the celebrated Bogoliubov dispersion relation

$$\begin{aligned}E_{\mathrm{B}}(k) &= \sqrt{\frac{\hbar^2\,k^2}{2\,m}\left(\frac{\hbar^2\,k^2}{2\,m} + 2\,g n_0\right)}, \quad \text{hence} \\ u(k) \pm v(k) &= \left[\frac{\hbar^2\,k^2/(2\,m)}{E_{\mathrm{B}}(k)}\right]^{\pm 1/2} \quad \text{and} \\ \hat{K}_{\mathrm{B}} &= E_0 + \sum_{\mathbf{k}\neq 0} E_{\mathrm{B}}(k)\,\hat{b}^\dagger(\mathbf{k})\,\hat{b}(\mathbf{k}).\end{aligned}$$

We will not tackle the calculation of E_0, which suffers from a subtle—but unphysical—ultraviolet divergence. This divergence originates from the approximation of $V(|\mathbf{r} - \mathbf{r}'|)$ by a δ-peak and may be cured by means of a suitable renormalization of the ground state, for instance detailed in Cohen-Tannoudji's lectures at the Collège de France (available on the Internet).

11 The final result for $\hat{K}_{\mathrm{B}}$ has a deep physical meaning. Comment.

12 Express $E_{\mathrm{B}}(k)$ in the form

$$E_{\mathrm{B}}(k) = g n_0 \sqrt{\frac{k^2\,\xi^2}{2}\left(\frac{k^2\,\xi^2}{2} + 2\right)}, \quad \text{where} \quad \xi = \frac{\hbar}{\sqrt{m\,g n_0}}$$

is called the healing length. Show that the quantum fluctuations of the homogeneous system are phonons (sound waves) in the low-wavenumber limit $k\,\xi \ll 1$, and (gapped) free particles when $k\,\xi \gg 1$. Plot $E_{\mathrm{B}}(k)$ as a function of k.

Quantum Depletion of the Condensate and One-Body Density Matrix

13 The average value of some quantum operator $\hat{f}$ in the statistical ensemble with grand-canonical Hamiltonian $\hat{K}_{\mathrm{B}}$ is defined as

$$\langle \hat{f} \rangle = \frac{\mathrm{tr}\{\hat{f} \exp[-\hat{K}_{\mathrm{B}}/(k_{\mathrm{B}} T)]\}}{\mathrm{tr}\{\exp[-\hat{K}_{\mathrm{B}}/(k_{\mathrm{B}} T)]\}},$$

where k_{B} is the Boltzmann constant. Verify that

$$\langle \hat{b}^\dagger(\mathbf{k})\, \hat{b}(\mathbf{k}') \rangle = n(k)\, \delta_{\mathbf{k},\mathbf{k}'}, \quad \langle \hat{b}(\mathbf{k})\, \hat{b}^\dagger(\mathbf{k}') \rangle = [1 + n(k)]\, \delta_{\mathbf{k},\mathbf{k}'}, \quad \text{and} \quad \langle \hat{b}(\mathbf{k})\, \hat{b}(\mathbf{k}') \rangle = 0,$$

where $n(k)$ is to determine as a function of $E_{\mathrm{B}}(k)$ and $k_{\mathrm{B}} T$. What does $n(k)$ equal to when $T = 0$?

14 Express the number of atoms with wavevector $\mathbf{k} \neq 0$,

$$N(k) = \langle \hat{a}^\dagger(\mathbf{k})\, \hat{a}(\mathbf{k}) \rangle,$$

as a function of $u(k)$, $v(k)$, and $n(k)$.

15 Show that the depletion of the condensate,

$$\delta N = \sum_{\mathbf{k} \neq 0} N(k),$$

is nonzero at $T = 0$. This result is very surprising. Comment.

16 The degree of quantum coherence of the system is characterized by its one-body density matrix

$$n^{(1)}(\mathbf{r}, \mathbf{r}') = \langle \hat{\Psi}^\dagger(\mathbf{r})\, \hat{\Psi}(\mathbf{r}') \rangle.$$

Show that

$$n^{(1)}(\mathbf{r}, \mathbf{r}') = n_0 + \frac{1}{L^3} \sum_{\mathbf{k} \neq 0} N(k)\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}.$$

How does this equation make it possible to extract δN? After replacing the sum over $\mathbf{k} \neq 0$ by an integral, demonstrate that

$$n^{(1)}(\mathbf{r}, \mathbf{r}') = n_0 + O\left(\frac{1}{|\mathbf{r} - \mathbf{r}'|^2}\right) \quad \text{as} \quad |\mathbf{r} - \mathbf{r}'|/\xi \gg 1.$$

Conclude on the long-range coherence of the quantum many-body system.