Année universitaire 2024/2025
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TD1 : Coherent states, phase and number operators

1 Harmonic oscillator and coherent states

Consider a one-dimensional harmonic oscillator with Hamiltonian $\hat{\mathcal{H}} = \hat{p}^2/(2m) + (1/2)\, m\omega^2\hat{x}^2$.

1.1

Introducing the dimensionless variables :

$$\hat{X} = \sqrt{\frac{m\omega}{\hbar}}\hat{x} \qquad \hat{P} = \frac{1}{\sqrt{m\hbar\omega}}\,\hat{p} \tag{1}$$

and the transformation

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{X} + i\hat{P}) \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{X} - i\hat{P}) \tag{2}$$

show the following results :

$$\hat{\mathcal{H}} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2) \qquad [\hat{a}, \hat{a}^\dagger] = 1 \qquad [\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0 \tag{3}$$

knowing that $[\hat{x}, \hat{p}] = i\hbar$.

1.2

Verify that the Hamiltonian eigenstates admit the form

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \tag{4}$$

and find the corresponding eigenvalue. Show that the position-momentum uncertainty relation for the Hamiltonian eigenstates reads :

$$(\Delta X \Delta P)_n = n + 1/2 \tag{5}$$

1.3

We introduce the *coherent states* as eigenstates of the destruction operator

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \tag{6}$$

where α is a *complex* variable.
Calculate the uncertainty product $(\Delta X \Delta P)_\alpha$: what can you conclude ?
Represent the "uncertainty volume" $\Delta X \Delta P$ in the complex plane of the α variable. Given the expectation values $\langle\alpha|\hat{X}|\alpha\rangle$, $\langle\alpha|\hat{P}|\alpha\rangle$ and the uncertainty relation, justify why these states are called "semi-classical".

2 Coherent states and number statistics

2.1

We now wish to write the coherent states on the *number* basis $|n\rangle$ as $|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle$. Show that the c_n coefficients satisfy the recursion relation

$$c_{n+1} = \frac{\alpha}{\sqrt{n+1}} c_n. \tag{7}$$

Starting from the c_0 coefficient, show that this relation is satisfied by

$$c_n = \frac{\alpha^n}{\sqrt{n!}}\, c_0 \ . \tag{8}$$

Show that $c_0 = \exp(-|\alpha|^2/2)$.

2.2

Show that the number distribution $P_\alpha(n) = |\langle n|\alpha\rangle|^2$ associated with a coherent state $|\alpha\rangle$ is the Poissonian distribution

$$P_\alpha(n) = e^{-\langle \hat{n}\rangle} \frac{\langle \hat{n}\rangle^n}{n!} \tag{9}$$

where $\langle \hat{n}\rangle = |\alpha|^2$. Show that variance is $\Delta n^2 = \langle \hat{n}\rangle$.

2.3

Justify that the coherent states can be written in the form

$$|\alpha\rangle = e^{-|\alpha|^2/2}\, e^{\alpha \hat{a}^\dagger}|0\rangle \tag{10}$$

where the exponential of an operator is defined via the Taylor expansion

$$e^{\alpha \hat{a}^\dagger} = \sum_{n=0}^{\infty} \frac{(\alpha \hat{a}^\dagger)^n}{n!} \quad . \tag{11}$$

3 Phase operator and phase-number uncertainty

In analogy with complex numbers, we introduce the polar decomposition of the destruction operator

$$\hat{a} = e^{i\hat{\phi}} \hat{n}^{1/2} \tag{12}$$

where

$$\hat{n}^{1/2} = \sum_{n=0}^{\infty} n^{1/2}|n\rangle\langle n| \qquad e^{i\hat{\phi}} = \sum_{n=0}^{\infty} |n\rangle\langle n+1| \tag{13}$$

3.1

Show that $\hat{\phi}$ is not Hermitian, because $e^{i\hat{\phi}}$ is not a unitary operator, $(e^{i\hat{\phi}})^\dagger e^{i\hat{\phi}} \neq 1$. What would happen if the sum started from $n = -\infty$?

3.2

Show that

$$|\phi\rangle = \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} e^{in\phi}|n\rangle \tag{14}$$

is an eigenstate of the operator $e^{i\hat{\phi}}$ with eigenvalue $e^{i\phi}$. Can you draw an analogy between the $|n\rangle$ and $|\phi\rangle$ states on the one side, and momentum vs. position eigenstates on the other side ? What can you guess for the commutation relation $[\hat{n}, \hat{\phi}]$?

3.3

Show that

$$[\hat{n}, e^{i\hat{\phi}}] = -e^{i\hat{\phi}} \tag{15}$$

By Taylor-expanding the exponential on both sides, show that above commutator is compatible with the commutation relation

$$[\hat{n}, \hat{\phi}] = i \quad . \tag{16}$$

This implies the phase-number uncertainty relation $\boxed{\Delta n \Delta\phi \gtrsim 1/2}$, which will be *fundamental* for this course.

4 Phase-number uncertainty for coherent states

We now consider the phase statistics associated with a coherent state.

4.1

Show that the phase distribution $P_\alpha(\phi) = |\langle\phi|\alpha\rangle|^2$ is given by

$$P_\alpha(\phi) = \frac{e^{-|\alpha|^2}}{2\pi} \left| \sum_n \frac{(e^{-i\phi}\alpha)^n}{\sqrt{n!}} \right|^2 \tag{17}$$

and justify why the maximum probability is associated with $\phi = \theta$, where $\alpha = |\alpha|e^{i\theta}$.

4.2

Using the number representation of the phase operator

$$\langle n|\hat{\phi}|\alpha\rangle = -i\frac{\partial}{\partial n}\langle n|\alpha\rangle \tag{18}$$

and considering $|\alpha| \gg 1$, show that

$$\langle\alpha|\hat{\phi}|\alpha\rangle = \theta - \frac{i}{2}(\log\langle n\rangle - \langle\log n\rangle) \tag{19}$$

[Use the Stirling formula $n! \approx \sqrt{2\pi n}\ n^n\ e^{-n}$, and convince yourself that its use is justified by the fact that $|\alpha| \gg 1$]. For $|\alpha| \gg 1$ the Poissonian distribution for the number statistics has a vanishing relative uncertainty, namely $P_\alpha(n) \to \delta_{n,\langle n\rangle}$. Justify in this limit that $\langle\hat{\phi}\rangle \approx \theta$.

4.3

Using the same assumptions as before, show that

$$\langle\alpha|\hat{\phi}^2|\alpha\rangle \approx \theta^2 + \frac{1}{2\langle n\rangle} \tag{20}$$

Conclude that, for a coherent state

$$\Delta\phi^2 \approx \frac{1}{2\langle n\rangle} \tag{21}$$

and, therefore, $\Delta\phi\ \Delta n \approx 1/\sqrt{2}$. Looking at the uncertainty volume in the complex plane α, as at Question 1.3), can one justify this result (roughly) with a simple geometrical argument valid in the limit $|\alpha| \gg 1$?

5 Phase correlations

Imagine to have a system of N independent harmonic oscillators. We are interested in the correlation function $\langle a_i^\dagger a_j\rangle$ associated with the i-th and j-th harmonic oscillator.

5.1

Imagine that each harmonic oscillator is in a different coherent state $|\alpha_i\rangle$, $i = 1, ..., N$, with $|\alpha_i| = |\alpha|$ for all i. Consider the quantity

$$I = \frac{1}{N} \sum_{ij} \langle a_i^\dagger a_j \rangle \quad . \tag{22}$$

Show that I is extensive, $I = N|\alpha|^2 = N_{\rm tot}$ (total average boson number), if the phases θ_i of the α_i's are all the same (*phase coherence*), while I is intensive, $I = |\alpha|^2$ (average boson number density), if the phases are completely random (*phase incoherence*).

5.2

Imagine now that all harmonic oscillators are in a Fock state, $|n_i\rangle$. Calculate I and show that it corresponds to the phase incoherent case. Can you justify this result from the number-phase uncertainty ?

6 Coherent states of fermionic pairs

Consider a fermion which can occupy two single-particle spin states, $|\uparrow\rangle$ and $|\downarrow\rangle$, with associated fermionic creation and destruction operators $\hat{a}_\sigma$, $\hat{a}_\sigma^\dagger$ ($\sigma = \uparrow, \downarrow$), satisfying fermionic anti-commutation relations $\{\hat{a}_\sigma, \hat{a}_{\sigma'}^\dagger\} = \delta_{\sigma,\sigma'}$, $\{\hat{a}_\sigma, \hat{a}_{\sigma'}\} = \{\hat{a}_\sigma^\dagger, \hat{a}_{\sigma'}^\dagger\} = 0$.

6.1

We introduce the *pair operators* $b_p = \hat{a}_\downarrow \hat{a}_\uparrow$, $b_p^\dagger = \hat{a}_\uparrow^\dagger \hat{a}_\downarrow^\dagger$. Show that $[b_p, b_p] = [b_p^\dagger, b_p^\dagger] = 0$, but $[b_p, b_p^\dagger] = 1 - \hat{a}_\uparrow^\dagger \hat{a}_\uparrow - \hat{a}_\downarrow^\dagger \hat{a}_\downarrow$, so that the b_p, $b_p^\dagger$ operators realize only *partially* the algebra of bosonic operators.

6.2

Consider the coherent states of fermionic pairs, defined as

$$|\alpha\rangle = \mathcal{N} e^{\alpha \hat{a}_\uparrow^\dagger \hat{a}_\downarrow^\dagger} |0\rangle \tag{23}$$

where $\mathcal{N}$ is a normalization factor to be determined. Write the state in terms of fermionic Fock states. Show that

$$|\alpha\rangle = \frac{1}{\sqrt{1 + |\alpha|^2}} (1 + \alpha\ \hat{a}_\uparrow^\dagger \hat{a}_\downarrow^\dagger) |0\rangle \tag{24}$$

s

6.3

Calculate the expectation values $\langle \hat{n}_\uparrow + \hat{n}_\downarrow \rangle$ and $\langle (\hat{n}_\uparrow + \hat{n}_\downarrow)^2 \rangle$ and the particle-number variance. Show that the relative uncertainty on the total particle number has the same expression as for bosonic coherent states.

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TD2 : Ferromagnetism and spin waves

7 Heisenberg Hamiltonian, spin-to-boson mapping

In many ferromagnetic compounds, the interactions among magnetic moments $\boldsymbol{\mu}_i = g\mu_B \boldsymbol{S}_i$ are described by the Heisenberg Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{25}$$

where $J > 0$ is the exchange interaction, and the sum runs over the $\langle ij \rangle$ pairs of nearest neighbor on a hypercubic lattice in D dimensions (linear chain for $D = 1$, square lattice for $D = 2$, cubic lattice for $D = 3$, etc.) with lattice spacing a. The spin operators satisfy the commutation relations

$$[S_i^\alpha, S_j^\beta] = i\delta_{ij}\varepsilon_{\alpha\beta\gamma}S_i^\gamma \qquad |\boldsymbol{S}_i|^2 = S(S+1) \tag{26}$$

where $\varepsilon_{\alpha\beta\gamma}$ is the totally anti-symmetric tensor. We recall as well the definition of the spin raising/lowering operators

$$S_i^+ = S_i^x + iS_i^y \qquad S_i^- = S_i^x - iS_i^y \tag{27}$$

and their action on an eigenstate of the S_i^z operator, $|S, m_S\rangle$

$$S_i^\pm |S, m_S\rangle = \sqrt{S(S+1) - m_S(m_S \pm 1)}\ |S, m_S \pm 1\rangle \quad . \tag{28}$$

7.1

Show that

$$S_i^x S_j^x + S_i^y S_j^y = \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) \ . \tag{29}$$

On the basis of the rotation symmetry of the left-hand side, justify on physical grounds why the right-hand side does not contain operator products of the kind S^+S^+ or S^-S^-.

7.2

Show that the state $|\Psi_0\rangle = \otimes_{i=1}^N |S, m_S = S\rangle_i$ is an eigenstate of $\mathcal{H}$, with energy $E_0 = -NJzS^2/2$, where $z = 2D$ is the coordination number of the lattice (number of nearest neighbors).

7.3

We now want to show that $|\Psi_0\rangle$ is also the *ground* state of $\mathcal{H}$. We introduce the magnetization $M = \sum_i S_i^z$. Justify that $[\mathcal{H}, M] = 0$ (you can do the explicit calculation, or use a simple symmetry argument).
Therefore the eigenstates of $\mathcal{H}$ are also eigenstates of M. If $|\Psi_0\rangle$ is the only eigenstate of M with eigenvalue NS, the eigenstates of M with eigenvalue $NS - 1$ are N-times degenerate. Indeed one can take a state such as

$$|\Psi_1^{(i)}\rangle = S_i^-|\Psi_0\rangle \quad . \tag{30}$$

Show that

$$\mathcal{H}|\Psi_1^{(i)}\rangle = (E_0 + zJS)|\Psi_1^{(i)}\rangle - JS\sum_d |\Psi_1^{(i+d)}\rangle \tag{31}$$

where $\sum_d$ runs over the nearest neighbors.

7.4

Changing the basis in the subspace of states with magnetization $M = NS - 1$, we define the states

$$|\Psi_1^{(\boldsymbol{q})}\rangle = \frac{1}{\sqrt{N}} \sum_i e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i} |\Psi_1^{(i)}\rangle \quad . \tag{32}$$

Show that $\mathcal{H}|\Psi_1^{(\boldsymbol{q})}\rangle = (E_0 + \epsilon_q)|\Psi_1^{(\boldsymbol{q})}\rangle$ where

$$\epsilon_q = JzS(1-\gamma_{\boldsymbol{q}}) \qquad \gamma_{\boldsymbol{q}} = \frac{1}{z}\sum_d e^{i\boldsymbol{q}\cdot\boldsymbol{d}} = \frac{2}{z}\sum_{i=x,y,..} \cos(q_i a) \tag{33}$$

(the $\boldsymbol{d}$ vectors connect a site to its z nearest neighbors, and $\sum_{i=x,y,...}$ runs over the components of the wavector $\boldsymbol{q}$ in D dimensions).
Conclude that $|\Psi_0\rangle$ is one of the ground states of $\mathcal{H}$ in the magnetization sectors $M = NS, NS-1$. Justify qualitatively that the states with magnetiazation $NS-2$, $NS-3$, etc. have an even larger energy.

7.5

Show that in the $q \to 0$ limit, $\epsilon_q \approx JSa^2q^2$. Therefore the dispersion relation ϵ_q strongly resembles that of free particles.
In the following we shall make this link explicit, transforming the spin model into a model of bosonic particles. We introduce the Holstein-Primakoff (HP) transformation from spins to bosons :

$$S^+ = f(n)\,\sqrt{2S}\;a \qquad S^- = \sqrt{2S}\;a^\dagger\;f(n) \qquad S^z = S - n \tag{34}$$

where $n = a^\dagger a$, $f(n) = \left(1 - \frac{n}{2S}\right)^{1/2}$, and a, $a^\dagger$ are bosonic operators, satisfying the commutation relation $[a, a^\dagger] = 1$.
We would like to show that this transformation is canonical, namely that it respects the commutation rules of spin operators. First of all, verify that, for spin operators defined as in Eq. (**??**),

$$[S^+, S^-] = 2S^z\ . \tag{35}$$

To check that the HP transformation verifies this commutation relation, show that

$$a\;n = (n+1)\;a \qquad a^\dagger n = (n-1)\;a^\dagger\ . \tag{36}$$

Convince yourself that this entails

$$a\;f(n) = f(n+1)\;a \qquad a^\dagger f(n) = f(n-1)\;a^\dagger \tag{37}$$

and conclude that S^+ et S^-, defined as in Eq. (**??**), satisfy Eq. (**??**).

8 Thermodynamics of spin waves, Bloch's $T^{3/2}$ law

8.1

If we focus on the lowest-energy eigenstates (ground state and first excited states), we have that $\langle S_i^z\rangle = S - \langle n_i\rangle \approx S$ – as we have seen it in the previous section. This implies that for these states $\langle n_i\rangle \ll 2S$, namely the bosons form a very diluted gas. This justifies that we *linearize* the HP transformation as follows

$$S_i^+ \approx \sqrt{2S}a_i \quad S_i^- \approx \sqrt{2S}a_i^\dagger\ . \tag{38}$$

Neglecting terms of order n_i^2, rewrite the Hamiltonian in terms of bosonic operators, and show that it describes a gas of free bosonic quasi-particles (*magnons*), whose dispersion relation is given by ϵ_q.

8.2

The magnetization per spin

$$m = \frac{\langle M \rangle}{N} = S - \frac{1}{N}\sum_i \langle n_i \rangle \tag{39}$$

is related to the density of magnons. Using Bose-Einstein statistics, show that for $T \ll JzS$ in D dimensions,

$$m(T) = S - \frac{\Omega_D}{2(2\pi)^D}\left(\frac{k_B T}{JS}\right)^{D/2} \Gamma(D/2)\; g_{D/2}(1) \tag{40}$$

where

$$\Gamma(D/2)\; g_{D/2}(1) = \int_0^\infty dx\; \frac{x^{D/2-1}}{e^x - 1} \tag{41}$$

and Ω_D is the solid angle in D dimensions. For $D = 3$ show that

$$m(T) = m(T=0)\left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right] \tag{42}$$

where T_c is to be determined [you can use the fact that $\Gamma(3/2)\; g_{D/2}(1) = 2.612\sqrt{\pi}/2$].

8.3

Is there a Bose-Einstein condensate of magnons in the system ? If not, why ?
Show that the product $\Gamma(D/2)\; g_{D/2}(1)$ diverges for $D < 3$. Can we have Heisenberg ferromagnetism at finite temperature for $D = 1, 2$? Can you link this result to the absence of condensation in an ideal Bose gas in $D = 1, 2$?

8.4

The above behavior of the magnetization is rather different from that predicted by mean-field theory, that we have examined (or will examine) in class. Within mean-field theory one has that $m(T)$ (dimensionless magnetization) satisfies the self-consistent equation

$$m = S\; \mathcal{B}_S(\beta J S m) \tag{43}$$

where $\beta = 1/(k_B T)$ and $\mathcal{B}_S(x)$ is the Brillouin function

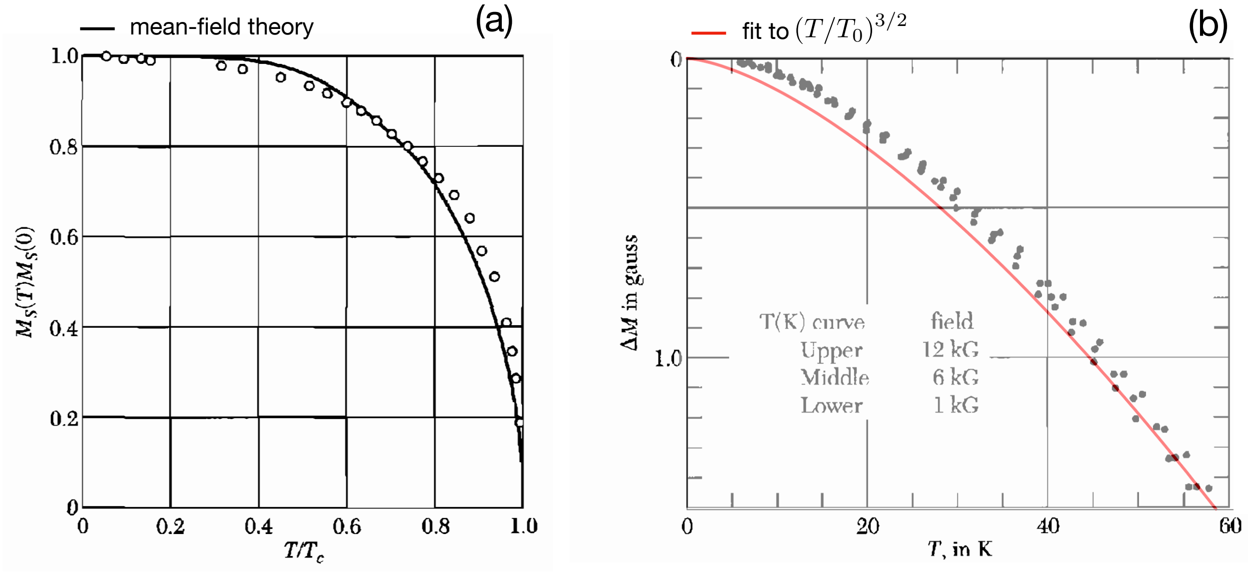
$$\mathcal{B}_S(x) = \frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}\; x\right) - \frac{1}{2S}\coth\left(\frac{1}{2S}\; x\right) \; . \tag{44}$$

Show that in the low-temperature limit $\beta \to \infty$, $m = S$. Considering instead low (but finite) temperatures $\beta J S^2 \gg 1$, we can expand the $\coth(x)$ function as $1 + 2e^{-2x} + ...$ Conclude that, within mean-field theory

$$m(T) \approx m(T=0) - \frac{1}{2}e^{-\beta J S} \; . \tag{45}$$

8.5

Fig. **??** shows the magnetization of Nickel as a function of temperature, compared to mean-field theory and spin-wave theory. What can you conclude ?



Nickel: $T_c = 627K$

FIGURE 1 – Magnetization of Ni as a function of temperature : (a) experimental data compared to mean-field theory (data from P. Weiss and R. Forrer) ; (b) experimental data at low temperature for $\Delta M = M(0) - M(T)$ fitted to the $T^{3/2}$ law (exp. data from B. E. Argyle, S. H. Charap and E. W. Pugh, Phys. Rev. 132, 2051 (1963)).

8.6

The analogy with Bose-Einstein condensation in the example given so far is not complete – as you may have remarked in replying to the question **??**. On the other hand, another model of magnetism allows for a closer connection with a system of bosons : the so-called XY model $\mathcal{H} = -J\sum_{ij}\left(S_i^x S_j^x + S_i^y S_j^y\right)$. To a first approximation the ground state of this model can be viewed as a collection of spins pointing along *e.g.* the x axis, $\langle S_i^x\rangle = S$. Justify that $\langle S_i^z\rangle = 0$ so that $\langle n_i\rangle = S$, and $\langle (S_i^z)^2\rangle = \langle n_i^2\rangle - \langle n_i\rangle^2 = S/2$.
Conclude that one can take $n_i \approx \langle n_i\rangle$ in the limit $S \gg 1$. Rewrite the spin operators in terms of HP bosons (Eq. (**??**)) in this approximation, and establish a relationship between the S^x and S^y operators and the phase operator ϕ for the bosons (as seen in the TD no. 1), defined such that $a = e^{i\phi}\sqrt{n}$.

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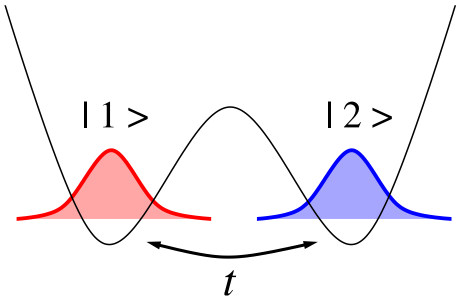
TD3 : Bosons in a double-well potential

In this TD we will investigate the physics of N identical bosons trapped in a double-well potential (bosonic Josephson junction). In the limit of a very deep potential, we can consider only two orthonormal single-particle states, $|1\rangle$ and $|2\rangle$, localized on the two sides of the double-well potential.
The many-body Hamiltonian on this reduced basis takes the form :

$$\hat{\mathcal{H}} = -t\left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1\right) + \frac{U}{2}\left[\hat{n}_1\left(\hat{n}_1 - 1\right) + \hat{n}_2\left(\hat{n}_2 - 1\right)\right] \tag{46}$$

where $\hat{a}_1, \hat{a}_1^\dagger$ and $\hat{a}_2, \hat{a}_2^\dagger$ are bosonic creation/destruction operators.



9 Many-body states : Fock states, Schrödinger's cat states and BEC states.

In this section we consider trial wave-functions to describe the ground state of the model.

9.1

Consider the Fock state

$$|N_1, N_2\rangle = \frac{\left(\hat{a}_1^\dagger\right)^{N_1}}{\sqrt{N_1!}} \frac{\left(\hat{a}_2^\dagger\right)^{N_2}}{\sqrt{N_2!}} |0\rangle \tag{47}$$

Write down its one-body density matrix $g_{ij}^{(1)} = \langle \hat{a}_i^\dagger \hat{a}_j \rangle$. For what values of N_1 and N_2 is the system showing condensation/fragmentation ?

9.2

Consider then the *Schrödinger's cat* state

$$|N_1, N_2; N_2, N_1\rangle = \frac{1}{\sqrt{2}}\left(|N_1, N_2\rangle + |N_2, N_1\rangle\right) \tag{48}$$

Calculate its one-body density matrix $g_{ij}^{(1)}$ for $|N_1 - N_2| > 1$; can this state show condensation ?

9.3

We then take the BEC state

$$|\alpha,\phi\rangle = \frac{1}{\sqrt{N!}}\left(\frac{\hat{a}_1^\dagger + \alpha e^{i\phi}\ \hat{a}_2^\dagger}{\sqrt{1+\alpha^2}}\right)^N |0\rangle \tag{49}$$

Write down its one-body density matrix $g_{ij}^{(1)}$. To do so, it can be useful to introduce the orthonormal states

$$|+\rangle = \frac{|1\rangle + \alpha e^{i\phi}\ |2\rangle}{\sqrt{1+\alpha^2}} \qquad |-\rangle = \frac{\alpha|1\rangle - e^{i\phi}\ |2\rangle}{\sqrt{1+\alpha^2}} \tag{50}$$

and the associated creation/destruction operators $\hat{a}_\pm$, $\hat{a}_\pm^\dagger$. Diagonalise $g_{ij}^{(1)}$ and show that the state corresponds to a perfect condensate (as it was obvious from the first definition....).

9.4

Show that the Fock state can be obtained by Fourier transformation of the BEC state with respect to ϕ. Conclude on the existence of a phase-difference/number-difference uncertainty.

10 Variational determination of the ground state

10.1

Calculate the energy expectation value for the Fock state $E(N_1,N_2) = \langle N_1,N_2|\hat{\mathcal{H}}|N_1,N_2\rangle$, and for the Schödinger's cat state. Find the combination (N_1,N_2) minimizing the energy in the case of repulsive $(U>0)$ and attractive $(U<0)$ interactions. Is the Fock state with $N_1 \neq N_2$ an acceptable equilibrium state of the system ?

10.2

Calculate the energy expectation value for the BEC state $E(\alpha,\phi)$, and show that the energy is an explicit function of the phase ϕ. Assuming $\alpha = 1$, minimize with respect to ϕ for both attractive and repulsive interactions.

10.3

Comparing the minimum energies $E_{\rm min}(N_1,N_2)$ and $E_{\rm min}(\alpha=1,\phi)$, determine the transition points between fragmented states and condensate states upon varying the ratio U/t. Draw the corresponding phase diagram on the U/t axis.

11 Schwinger pseudo-spin representation

11.1

Introducing the operators

$$\hat{J}_x = \frac{1}{2}\left(\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\right) \qquad \hat{J}_y = \frac{1}{2i}\left(\hat{a}_1^\dagger\hat{a}_2 - \hat{a}_2^\dagger\hat{a}_1\right) \qquad \hat{J}_z = \frac{1}{2}\left(\hat{a}_1^\dagger\hat{a}_1 - \hat{a}_2^\dagger\hat{a}_2\right) \tag{51}$$

show that they satisfy the commutation relations of angular momentum, $[\hat{J}_\alpha,\hat{J}_\beta] = i\varepsilon^{\alpha\beta\gamma}\hat{J}_\gamma$.

11.2

Calculating $J^2 = |\hat{\boldsymbol{J}}|^2$, determine the effective spin length. Show that the Hamiltonian of the system in the pseudospin variables takes the form

$$\hat{\mathcal{H}} = -2t\hat{J}_x + U\left(\hat{J}_z^2 + J^2 - N\right) \quad . \tag{52}$$

Treating the J_α operators as classical variables, what are the values of the spin components which minimize the energy in the opposite limits $|U|/t \ll 1$, $U/t \gg 1$ and $-U/t \gg 1$?

11.3

Calculate the vector $\langle\hat{\boldsymbol{J}}\rangle = (\langle\hat{J}_x\rangle, \langle\hat{J}_y\rangle, \langle\hat{J}_z\rangle)$ for the Fock state $|N_1, N_2\rangle$ and the BEC state $|\alpha, \phi\rangle$. Introducing the angle variable θ such that

$$\frac{1}{\sqrt{1+\alpha^2}} = \cos(\theta/2) \qquad \frac{\alpha}{\sqrt{1+\alpha^2}} = \sin(\theta/2) \tag{53}$$

show that the state vector $\langle\hat{\boldsymbol{J}}\rangle$ for the BEC state is a vector of length N with polar/azimuthal angles ϕ, θ. Represent the ground state of the system in the various phases, as determined in the previous section, via the length and orientation of the state vector.

12 Momentum distribution in the BEC state

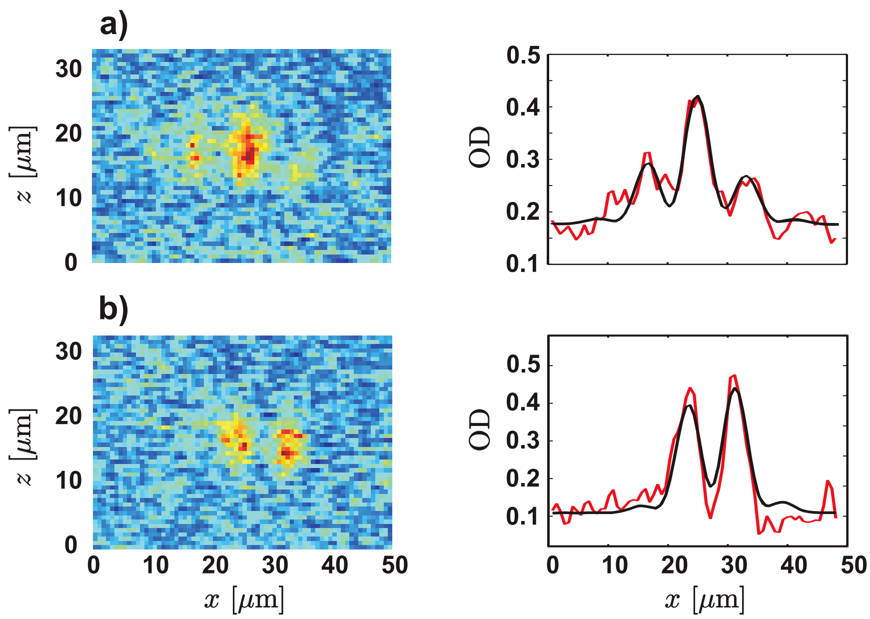


FIGURE 2 – Absorption images of bosons released from a double-well trap. From M. Albiez's PhD thesis, University of Heidelberg (2005).

Be $\Phi_1(x)$ and $\Phi_2(x)$ the spatial wavefunction associated with the two states $|1\rangle$ and $|2\rangle$, with the property $\Phi_2(x) = \Phi_1(x-d)$ (d = separation between the two wells). The states Φ_1 and Φ_2 are part of a basis Φ_i of orthonormal wavefunctions.

12.1

Calculate $\langle\hat{\psi}^\dagger(x)\hat{\psi}(x')\rangle$ for the generic BEC state $|\alpha, \phi\rangle$.
(*Suggestion* : expand the field operators on the Φ_i basis).

12.2

Calculate the momentum distribution $n(k) = \langle \hat{a}_k^\dagger \hat{a}_k \rangle$, where

$$a_k = \int dx \, \frac{e^{-ikx}}{\sqrt{V}} \, \psi(x) \; . \tag{54}$$

You should find an expression containing N, α, ϕ, k and $\tilde{\Phi}_1(k)$ (Fourier transform of the Φ_1 wavefunction). In the case of Gaussian wavefunctions, $\Phi_1(x) \sim \exp[-x^2/(2\sigma^2)]$, sketch the form of $n(k)$.

12.3

Fig. 1 shows the measurement of the momentum distribution of bosons trapped in double well potential for two different measurement shots. Can you tell the phase difference ϕ between the two wells in the two cases ?

TD4 : Applications of the Gross-Pitaevskii equation

In this TD we will concentrate on the study of the Gross-Pitaevskii equation (GPE) for a contact potential :

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\rm ext}(\boldsymbol{r}) + g|\Psi_0(\boldsymbol{r})|^2\right)\Psi_0(\boldsymbol{r}) = \mu\Psi_0(\boldsymbol{r}) \tag{55}$$

for the study of inhomogeneous condensates.

13 Derivation of the Gross-Pitaevskii equation : variational approach

13.1

We postulate that the state of the system is a perfect condensate in the single-particle wavefunction $\chi_0(\boldsymbol{r})$

$$|\Psi\rangle = \frac{(\hat{a}_0^{+})^N}{\sqrt{N!}}|0\rangle \tag{56}$$

where

$$\hat{a}_0^\dagger = \int d^d r\ \chi_0(\boldsymbol{r})\ \hat{\psi}^\dagger(\boldsymbol{r})\ . \tag{57}$$

Considering that in general

$$\hat{\psi}(\boldsymbol{r}) = \sum_\alpha \chi_\alpha(\boldsymbol{r})\ \hat{a}_\alpha \tag{58}$$

where $\chi_\alpha(\boldsymbol{r})$ are at set of orthonormal wavefunctions, containing $\chi_0(\boldsymbol{r})$, show that

$$\langle\Psi|\hat{\psi}^\dagger(\boldsymbol{r})D(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})|\Psi\rangle = N\ \chi_0^*(\boldsymbol{r})D(\boldsymbol{r})\chi_0(\boldsymbol{r}) \tag{59}$$

where $D(\boldsymbol{r})$ is a generic differential operator dependent on the position $\boldsymbol{r}$.
By the same token, show that

$$\langle\Psi|\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r})|\Psi\rangle = N(N-1)\ |\chi_0(\boldsymbol{r})|^2\ |\chi_0(\boldsymbol{r}')|^2\ . \tag{60}$$

13.2

In which limit do the above results coincide with the Bogolyubov replacement $\hat{\psi}(\boldsymbol{r}) \to \Psi_0(\boldsymbol{r})$? And how are Ψ_0 and χ_0 related ? Comment on the necessity of considering a spontaneous breaking of particle-number conservation (namely the fact that $\langle\hat{\psi}\rangle \neq 0$) when dealing with condensates.

13.3

Consider the many-body grand-canonical Hamiltonian

$$\begin{aligned}\hat{\mathcal{H}} - \mu\hat{N} &= \int d^d r\ \hat{\psi}^\dagger(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\rm ext}(\boldsymbol{r}) - \mu\right)\hat{\psi}(\boldsymbol{r}) \\ &+ \frac{1}{2}\int d^d r \int d^d r'\ V(\boldsymbol{r}-\boldsymbol{r}')\ \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r})\end{aligned} \tag{61}$$

Calculate $E_{\rm GP}(\Psi_0, \Psi_0^*) = \langle\Psi|\hat{\mathcal{H}} - \mu\hat{N}|\Psi\rangle$.
The functional minimization of $E_{\rm GP}(\Psi_0, \Psi_0^*)$ with respect to Ψ_0 leads to the Gross-Pitaevskii equation, Eq. (**??**). Specify the form of the interparticle potential, $V(\boldsymbol{r}-\boldsymbol{r}')$, implied by Eq. (**??**).

14 Thomas-Fermi approximation

14.1

Be R the characteristic length scale for the variations of the macroscopic wavefunction

$$\frac{R^2\ \nabla^2\Psi_0}{\Psi_0} \sim 1 \quad . \tag{62}$$

Show that, if $R \gg \xi$ (where $\xi = \hbar/\sqrt{2gmn}$ is the healing length), the kinetic part of the GPE can be neglected with respect to the non-linear term.
Conclude that, under the above assumption (the so-called Thomas-Fermi approximation), the condensate density satisfies the simple equation

$$|\Psi_0(\boldsymbol{r})|^2 = n(\boldsymbol{r}) = \frac{\mu - V_{\rm ext}(\boldsymbol{r})}{g} \tag{63}$$

14.2

Consider the case of a confining harmonic potential, $V_{\rm ext} = (1/2)m\omega^2 r^2$. Draw the radial density profile $n(r)$, and calculate the radius of the condensate (Thomas-Fermi radius).
If N is the total number of particles, show that the related chemical potential is

$$\mu(N) = \left(\frac{15}{8}\frac{gN}{\pi}\right)^{2/5}\left(\frac{m\omega^2}{2}\right)^{3/5} \tag{64}$$

Calculate the compressibility, $\kappa = \partial N/\partial\mu$, and comment on its dependence on g.

15 Condensate at a hard-wall potential

15.1

Consider the hard-wall potential in one dimension

$$V_{\rm ext}(x) = \begin{cases} 0 & x \geq 0 \\ \infty & x < 0 \ . \end{cases} \tag{65}$$

What are the boundary conditions for the GPE at $x = 0$ and $x = \infty$?
Writing

$$\Psi_0 = \sqrt{n}\ f\left(\frac{x}{\sqrt{2}\ \xi}\right) \tag{66}$$

where $n = |\Psi_0(x \to \infty)|^2$, show that the GPE takes the form

$$\frac{d^2 f(y)}{dy^2} = -2(f - f^3) \tag{67}$$

where $y = x/(\sqrt{2}\ \xi)$. Show that $f(y) = \tanh(y)$ is a solution to the above equation. Draw the full solution to the GPE equation : do you understand why ξ is called the "healing" length ?

16 Vortex solution

We look now for a solution to the GPE with finite vorticity, in the absence of external potentials ($V_{\rm ext} = 0$). Taking a system with cylindrical symmetry, consider a macroscopic wavefunction of the form

$$\Psi_0(r, \phi, z) = |\Psi_0(r)|\ e^{ip\phi} \qquad p \in \mathbb{Z} \quad . \tag{68}$$

16.1

What is the angular momentum of this wavefunction ? Calculate the related velocity field

$$\boldsymbol{v}_s(\boldsymbol{r}) = \frac{\hbar}{m}\boldsymbol{\nabla} S(\boldsymbol{r}) \tag{69}$$

where S is the phase of the wavefunction.
Calculate the vorticity of the velocity field, and show that the vorticity is quantized. By using Stokes' theorem, show that

$$\boldsymbol{\nabla} \times \boldsymbol{v}_s(\boldsymbol{r}) = \frac{h}{m}\; p\; \delta^{(2)}(r)\; \boldsymbol{e}_z \quad . \tag{70}$$

16.2

Show that the GPE equation takes the form

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}\right)|\Psi_0| + \frac{\hbar^2}{2m}\frac{p^2}{r^2}|\Psi_0| + g|\Psi_0|^3 - \mu|\Psi_0| = 0 \tag{71}$$

Writing $|\Psi_0| = \sqrt{n} f(y)$ with $|\Psi_0(r \to \infty)| = \sqrt{n}$ and $y = r/\xi$, rewrite the GPE in the form

$$\left(\frac{d^2}{dy^2} + \frac{1}{y}\frac{d}{dy}\right) f + \left(1 - \frac{p^2}{y^2}\right) f - f^3 = 0 \tag{72}$$

16.3

For $y \to 0$, we look for a solution in the form $f \sim y^\alpha$. Show that this works if $\alpha = |p|$.
In the opposite limit, $y \to \infty$, show that the GPE equation reduces to the same form as that of the hard-wall potential.
Interpolating between the two limits, sketch the form of the radial wavefunction $|\Psi_0(r)|$. What is the characteristic size of the vortex core ?

16.4

To conclude, we calculate the energy of the solution to the GPE containing one quantized vortex. Knowing that the energy functional is given by

$$E = \int d^3r \left(\frac{\hbar^2}{2m}|\boldsymbol{\nabla}\Psi_0|^2 + \frac{g}{2}|\Psi_0|^4\right) \tag{73}$$

we consider a cylindrical sample, with radius R and height L. Show that the energy difference between the macroscopic wavefunction containing a vortex and the uniform wavefunction (without vortices) can be written as

$$E_v = \frac{L\pi\hbar^2 n}{m}\int_0^{R/\xi} dy\; y\left[\left(\frac{df}{dy}\right)^2 + \frac{p^2}{y^2}f^2 + \frac{1}{2}(f^4 - 1)\right] \tag{74}$$

To estimate this integral, we drastically approximate $f(y)$ with the function $f(y) = y$ for $y < 1$ and $f(y) = 1$ for $y \geq 1$. Show that this leads to the estimate

$$E_v \approx \frac{L\pi\hbar^2 n}{m} p^2 \ln\left(\frac{bR}{\xi}\right) \tag{75}$$

where $b = 2.3$ (The exact result gives the same form for the energy, but a different coefficient $b = 1.46$, so the above estimate is not that bad after all).
Explain the fact that the energy of the vortex diverges with the system size $L, R \to \infty$, although the vortex excitation only leads to a localized depletion in the density profile around the vortex core.

16.5

Imagine that the cylindrical bucket containing the condensate is put into rotation at an angular velocity Ω. In the rotating reference frame the Hamiltonian takes the form

$$\mathcal{H} = \mathcal{H}_0 - \Omega L_z \tag{76}$$

where $\mathcal{H}_0$ and L_z are the Hamiltonian and the angular momentum in the laboratory frame.
Show that for $\Omega > \Omega_c$ (to be determined) the vortex configuration becomes stable, so that vortices start to appear in the system.

17 Vortex-vortex interactions

Imagining to rotate the bucket even faster, we want to investigate whether the vortex we have created acquires a higher vorticity, or whether we add instead more vortices with unit vorticity to the system. To this end we need to calculate the interaction energy between two vortices with cores at a distance $d \gg \xi$.
In presence of two vortices the velocity field takes the form

$$\boldsymbol{v}_s = \frac{\hbar}{m}\frac{p_1}{r}\,\boldsymbol{e}_\phi^{(0)} + \frac{\hbar}{m}\frac{p_2}{r-d}\,\boldsymbol{e}_\phi^{(d)} = \boldsymbol{v}_0 + \boldsymbol{v}_d \tag{77}$$

where the $\boldsymbol{e}_\phi^{(0)}$ and $\boldsymbol{e}_\phi^{(d)}$ vectors are referred to cylindrical reference frames with origins at $r = 0$ and $r = d$ respectively.
Similarly to what seen at question **??** (but even more drastically) we neglect the spatial variation of the density of the condensate, and we take

$$\Psi(\boldsymbol{r}) \approx \sqrt{n}\, e^{iS(\boldsymbol{r})} \tag{78}$$

where $n =$ const., and $\boldsymbol{v}_s = (\hbar/m)\boldsymbol{\nabla}S$.

17.1

Starting from the energy function Eq. (**??**), show that the energy of two vortices contains three terms, out of which the vortex-vortex interaction term can be written as

$$E_{\text{int}} = mn \int d^3r\ \boldsymbol{v}_0 \cdot \boldsymbol{v}_d \quad . \tag{79}$$

17.2

If $r \gg d$ we have that $\boldsymbol{e}_\phi^{(0)} \approx \boldsymbol{e}_\phi^{(d)}$. Considering that $R \gg d$, the points with $r \gg d$ will dominate the above integral, so that we can take this approximation all over the volume of the system. In this case, show that

$$E_{\text{int}} \approx \frac{2L\hbar^2\pi n}{m} p_1 p_2 \ln\left(\frac{R}{d}\right) \quad . \tag{80}$$

Comment on the nature of the interaction.

17.3

Now we are ready to respond to the initial question : what happens when rotating the condensate faster and faster ? Compare the energy of a vortex with vorticity $p = 2$, $E_v(p = 2)$, with the energy of two vortices $2E_v(p = 1) + E_{\text{int}}$. Which solution is energetically favored ?

17.4

Let us look now at the experiment, shown in Fig. **??**. Can you interpret what you see in light of the previous results ? Can you understand the structure of the vortex arrays appearing in the system ?

Mathematical appendix

Gradient in cylindrical coordinates

$$\boldsymbol{\nabla} = \boldsymbol{e}_r \, \frac{\partial}{\partial r} \; + \; \boldsymbol{e}_\phi \, \frac{1}{r}\frac{\partial}{\partial \phi} \; + \; \boldsymbol{e}_z \, \frac{\partial}{\partial z} \tag{81}$$

Laplacian in cylindrical coordinates

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \tag{82}$$

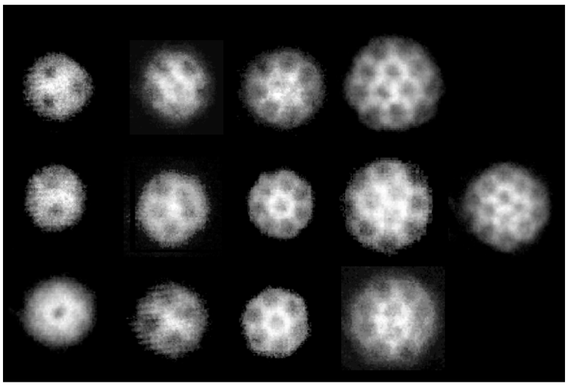
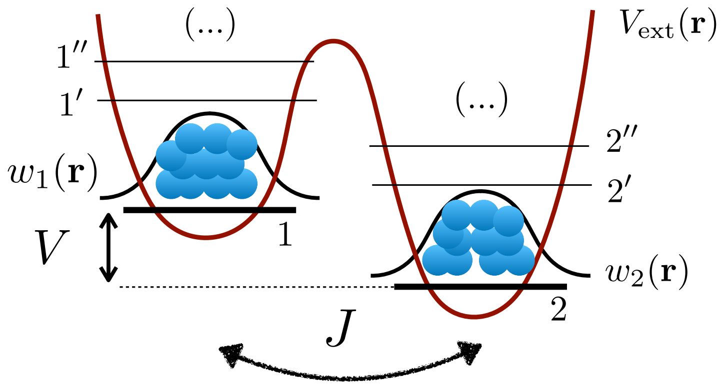


FIGURE 3 – Vortex arrays appearing in a condensate under rotation at increasing angular velocity. From F. Chevy's PhD thesis, ENS-Paris (2001).

TD5 : Josephson effects



In this exercise we will consider again the bosonic double well, this time with an energy offset between the two wells ; and we will obtain two fundamental equations for the evolution of the phase and number difference between the two wells – the so-called Josephson relations.
The general many-body Hamiltonian describing the system is

$$\hat{\mathcal{H}} = \int d^3r \; \hat{\psi}^\dagger(\boldsymbol{r}) \left[-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\boldsymbol{r}) \right] \hat{\psi}(\boldsymbol{r}) + \frac{g}{2} \int d^3r \; \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}) \tag{83}$$

where we have assumed a contact interaction $V(\boldsymbol{r}-\boldsymbol{r}') = g\delta(\boldsymbol{r}-\boldsymbol{r}')$ between the particles.

18 Equation of motion : Gross-Pitaevskii picture

In principle the field operator $\hat{\psi}(\boldsymbol{r})$ can be decomposed on the single-particle orthonormal states $w_\alpha(\boldsymbol{r}) = \langle \boldsymbol{r}|\alpha\rangle$:

$$\hat{\psi}(\boldsymbol{r}) = w_1(\boldsymbol{r})\hat{a}_1 + w_{1'}(\boldsymbol{r})\hat{a}_{1'} + ... + w_2(\boldsymbol{r})\hat{a}_2 + w_{2'}(\boldsymbol{r})\hat{a}_{2'} + ... \tag{84}$$

We assume that the states $w_\alpha(\boldsymbol{r})$ are localized on either side of the well. In general these states are *not* eigenstates of the one-body Hamiltonian $\mathcal{H}^{(1)} = -\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\boldsymbol{r})$; we can define nonetheless their average energies $E_\alpha = \langle\alpha|\mathcal{H}^{(1)}|\alpha\rangle$.
In the following we shall assume that the system is in a *condensate* state, which has support only on the *two lowest modes* $w_1(\boldsymbol{r})$ and $w_2(\boldsymbol{r})$, well localized on each side of the double well. As a consequence we can take

$$\hat{\psi}(\boldsymbol{r}) \approx w_1(\boldsymbol{r})\hat{a}_1 + w_2(\boldsymbol{r})\hat{a}_2 \; . \tag{85}$$

18.1

Inject the above truncated expression for the field operator into the many-body Hamiltonian, and show that it can be recast in the following form :

$$\hat{\mathcal{H}} = -J(\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1) + \frac{U}{2}\left(\hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_1\hat{a}_1 + \hat{a}_2^\dagger\hat{a}_2^\dagger\hat{a}_2\hat{a}_2\right) + V\hat{a}_1^\dagger\hat{a}_1 + ... \tag{86}$$

where J is the tunneling energy for going from one well to the next (so-called *Josephson energy*), U is the interaction energy among particles in the same well (the so-called *charging energy*) and V is a potential offset between the two wells.
Find the microscopic expression of the parameters J, V and U in terms of the functions $w_{1(2)}(\boldsymbol{r})$, and discuss which terms of the many-body Hamiltonian have been neglected.

18.2

Write the Heisenberg equations for the destruction operators

$$i\hbar \frac{d\hat{a}_1}{dt} = [\hat{a}_1, \hat{\mathcal{H}}] \qquad i\hbar \frac{d\hat{a}_2}{dt} = [\hat{a}_2, \mathcal{H}] \ . \tag{87}$$

Show that the replacement $\hat{a}_{1(2)} \to \Psi_{1(2)} \in \mathbb{C}$ gives rise to the (two-mode) Gross-Pitaevskii equation for this problem

$$\begin{aligned} i\hbar \frac{d\Psi_1}{dt} &= -J\Psi_2 + U|\Psi_1|^2\Psi_1 + V\Psi_1 \\ i\hbar \frac{d\Psi_2}{dt} &= -J\Psi_1 + U|\Psi_2|^2\Psi_2 \end{aligned} \tag{88}$$

Note : Here Ψ_1 and Ψ_2 are *not* to be interpreted as two different macroscopic wavefunctions, but as the amplitudes of the same macroscopic wavefunction on the two modes 1 and 2 on both sides of the double well, namely $\Psi_0(\boldsymbol{r}) = \Psi_1 w_1(\boldsymbol{r}) + \Psi_2 w_2(\boldsymbol{r})$.
As usual there exists a completely equivalent formulation in variational terms, which does not require to assume that the field operator takes a finite average value.

19 First Josephson relation

Write $\Psi_1 = A_1 e^{i\phi_1}$ and $\Psi_2 = A_2 e^{i\phi_2}$, with $A_{1(2)} = \sqrt{N_{1(2)}}$ the amplitude of the macroscopic wavefunction on each side of the well, and $N_{1(2)}$ the corresponding particle number.

19.1

Show that

$$\frac{dN_1}{dt} = \frac{d|\Psi_1|^2}{dt} = \frac{2JA_1A_2}{\hbar} \sin\Delta\phi = -\frac{dN_2}{dt} \tag{89}$$

where $\Delta\phi = \phi_1 - \phi_2$.
Therefore

$$\frac{d(\Delta N)}{dt} = \frac{4JA_1A_2}{\hbar} \sin\Delta\phi \tag{90}$$

where $\Delta N = N_1 - N_2$.

19.2

Conclude that (first Josephson relation)

$$I_{2\to 1} = I_c \sin\Delta\phi \tag{91}$$

where $I_{2\to 1}$ is the current of atoms going from well 2 to well 1 ; find an expression for the "critical current" I_c.

19.3

Show that at all times we can write

$$N_1(t) = \bar{N} + \frac{\Delta N(t)}{2} \qquad N_2(t) = \bar{N} - \frac{\Delta N(t)}{2} \tag{92}$$

where $\bar{N} = N/2$.
In the following we shall assume that $\Delta N \ll N$, namely the particle difference between the two wells is negligible compared to the total number of particles. This assumption can be justified in different ways : either there is a large offset V between the two wells preventing a large particle transfer from one well to the next ; or the charging energy U is significant, preventing too many particles to accumulate on one side only. Under this assumption, show that I_c is a constant up to $O(\Delta N/N)^2$ corrections.

20 Second Josephson relation

20.1

Write the derivatives $\frac{d}{dt}A_1 e^{i\phi_1}$, $\frac{d}{dt}A_2 e^{i\phi_2}$ using the Gross-Pitaevskii equations. Show that the two equations lead to the form

$$\frac{d(\Delta\phi)}{dt} = -\frac{V}{\hbar} - \frac{\Delta N}{N_1}\frac{d\phi_2}{dt} - \frac{U}{\hbar}\frac{N}{N_1}\Delta N \tag{93}$$

20.2

If the two modes $w_1(\boldsymbol{r})$ and $w_2(\boldsymbol{r})$ are extended (that is, their size grows with the particle number N), we have that $U \sim N^{-1}$ (see derivation of the microscopic parameters at the question **??**). Justify therefore that we end up with the (second Josephson) equation

$$\frac{d(\Delta\phi)}{dt} \approx -\frac{V}{\hbar} \tag{94}$$

up to terms of order $O(\Delta N/N)$.

20.3

Combining the two Josephson relations Eq. (**??**) and Eq. (**??**) show that a DC potential difference V leads to an AC current across the double well at frequency $V/\hbar$.

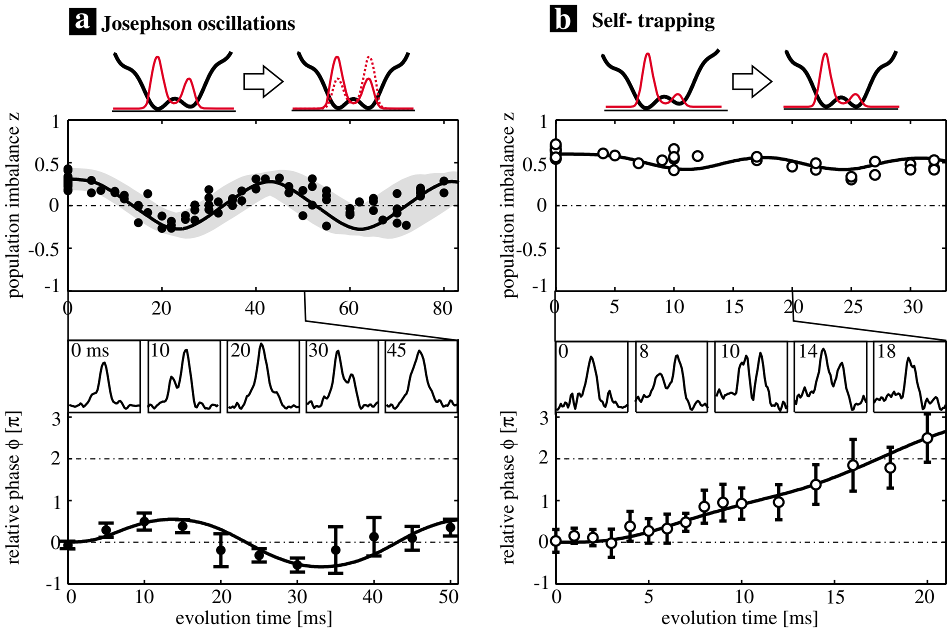


FIGURE 4 – Dynamics of a bosonic double well : here $\Delta N/N \to z$ and $(-\Delta\phi) \to \phi$. The density profiles in the middle panels are the interference patterns of the atoms after expansion. Figure taken from M. Albiez *et al.* Phys. Rev. Lett. **95**, 010402 (2005).

20.4

Fig. **??** shows the experimental results (using ultracold Rb atoms in an optical potential) for the dynamics of the population and phase differences ΔN and $\Delta\phi$ for a bosonic Josephson junction initialized with a small particle imbalance (first column) and with a large particle imbalance (second column), induced by a potential offset between the two wells, but then released during the evolution. Can you interpret the results you see using the Josephson relations (and also using some of the results you have obtained in TD 3) ? And is the experiment always conducted in the regime to which the above equations apply ?

The effects we have seen in this TD apply to all physical systems exhibiting condensation, namely developing a macroscopic wavefunction. These include not only ultracold atoms, but also superfluid ^{4}He, as well as superconducting systems. The Josephson effects appear whenever two condensates are put into contact via a so-called "weak link" or Josephson junction (namely a mechanism that lets particle tunnel from one condensate to the other, perturbing weakly each condensate). Josephson junctions are at the core of many devices based on superconducting circuits, such as some of the most sensitive magnetic field sensors.

TD6 : Interacting Bose fluids

21 Bogolyubov theory for the soft-disk gas

In this exercise we shall generalize Bogolyubov theory seen in the lectures to the case of a generic pair potential $V_{\rm int}(\boldsymbol{r}-\boldsymbol{r}')$. We shall introduce the following definitions for the potential and its Fourier transform $\tilde{V}_{\rm int}(\boldsymbol{q})$:

$$\tilde{V}_{\rm int}(\boldsymbol{q}) = \int d^3r \; e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \; V_{\rm int}(\boldsymbol{r}) \qquad V_{\rm int}(\boldsymbol{r}) = \frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \; \tilde{V}_{\rm int}(\boldsymbol{q}) \tag{95}$$

where $\mathcal{V}$ is the volume of the system.

21.1

Write Gross-Pitaevskii equation for the condensate wavefunction $\Psi_0(\boldsymbol{r})$ in the presence of the interaction potential $V_{\rm int}(\boldsymbol{r}-\boldsymbol{r}')$; show that the uniform condensate wavefunction

$$\Psi_0(\boldsymbol{r}) = \sqrt{n_0} = \sqrt{N_0/\mathcal{V}} \tag{96}$$

containing N_0 particles is a solution of the equation, with chemical potential

$$\mu = n_0 \tilde{V}_{\rm int}(\boldsymbol{q}=0) \; . \tag{97}$$

21.2

We shall now build Bogolyubov theory starting from this condensate wavefunction. We recall the Bogolyubov quadratic Hamiltonian

$$\begin{aligned}\hat{\mathcal{H}}_2 &= \sum_{\boldsymbol{q}\neq 0} (\epsilon_{\boldsymbol{q}} - \mu) \; \hat{a}^\dagger_{\boldsymbol{q}}\hat{a}_{\boldsymbol{q}} \\ &+ \frac{n_0}{2}\int d^3r \int d^3r' V_{\rm int}(\boldsymbol{r}-\boldsymbol{r}') \left(\delta\hat{\psi}(\boldsymbol{r})\delta\hat{\psi}(\boldsymbol{r}') + \text{h.c.} + 2\delta\hat{\psi}^\dagger(\boldsymbol{r})\delta\hat{\psi}(\boldsymbol{r}') + 2\delta\hat{\psi}^\dagger(\boldsymbol{r})\delta\hat{\psi}(\boldsymbol{r})\right)\end{aligned} \tag{98}$$

where

$$\delta\hat{\psi}(\boldsymbol{r}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\boldsymbol{q}\neq 0} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \; \hat{a}_{\boldsymbol{q}} \qquad \hat{a}_{\boldsymbol{q}} = \frac{1}{\sqrt{\mathcal{V}}}\int d^3r \; e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \; \delta\hat{\psi}(\boldsymbol{r}) \tag{99}$$

and $\epsilon_{\boldsymbol{q}} = \hbar^2 q^2/(2m)$.
Put the Hamiltonian in the form

$$\hat{\mathcal{H}}_2 = \frac{1}{2}\sum_{\boldsymbol{q}\neq 0} \begin{pmatrix} \hat{a}^\dagger_{\boldsymbol{q}} \\ \hat{a}_{-\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} A_{\boldsymbol{q}} & B_{\boldsymbol{q}} \\ B_{\boldsymbol{q}} & A_{\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} \hat{a}_{\boldsymbol{q}} \\ \hat{a}^\dagger_{-\boldsymbol{q}} \end{pmatrix} \tag{100}$$

and determine the $A_{\boldsymbol{q}}$, $B_{\boldsymbol{q}}$ coefficients.

21.3

The Bogolyubov quasi-particle spectrum is given by $E_{\boldsymbol{q}} = \sqrt{A^2_{\boldsymbol{q}} - B^2_{\boldsymbol{q}}}$. Show that

$$E_{\boldsymbol{q}} = \sqrt{\epsilon_{\boldsymbol{q}}\left(\epsilon_{\boldsymbol{q}} + 2n_0\tilde{V}_{\rm int}(\boldsymbol{q})\right)} \; . \tag{101}$$

What happens in the case of a contact potential $V_{\rm int}(\boldsymbol{r}-\boldsymbol{r}') = g \; \delta(\boldsymbol{r}-\boldsymbol{r}')$?

21.4

We shall now consider the soft-disk potential

$$V_{\text{int}}(\boldsymbol{r}-\boldsymbol{r}') = \begin{cases} V_0 & |\boldsymbol{r}-\boldsymbol{r}'| < R \\ 0 & \text{otherwise} \ . \end{cases} \tag{102}$$

We start by calculating its Fourier transform. Using polar coordinates, show that

$$\tilde{V}_{\text{int}}(\boldsymbol{q}) = 4\pi V_0 \int_0^R dr \ r^2 \ \frac{\sin(qr)}{qr} \tag{103}$$

and conclude that

$$\tilde{V}_{\text{int}}(\boldsymbol{q}) = \frac{4\pi V_0 R^3}{(qR)^3} \left[\sin(qR) - qR\cos(qR)\right] \ . \tag{104}$$

21.5

The dispersion relation can be written in the dimensionless form

$$e_x = \frac{2mR^2}{\hbar^2} E_{\boldsymbol{q}} = x\sqrt{x^2 + \frac{D}{x^3}\left(\sin x - x\cos x\right)} \ . \tag{105}$$

What is x ? Motivate why the parameter D can be interpreted as the ratio between the potential energy change when modifying the condensate wavefunction on the length scale of R, and the kinetic energy cost of introducing an inhomogeneity on the same length scale.

21.6

Plot the dispersion relation e_x for various values of D, and estimate numerically (i.e. approximately) the critical value D_{c1} at which a so-called *roton minumum* appears in the dispersion relation ; for which value of $x = x_{\text{rot}}$ does that occur ?

21.7

Increasing the value of D even further, estimate approximately the value D_{c2} at which the dispersion relation becomes *gapless* at the roton wavevector. What happens for $D > D_{c2}$? Is the uniform condensate wavefunction stable to small perturbations ? What would be in your opinion a stable solution ?

22 Condensate fraction for a hard-disk wavefunction

Following Penrose and Onsager (1956) we calculate the condensate fraction associated with a model wavefuction for ^{4}He (proposed originally by R. P. Feynman). Such wavefunction is the same as the "Boltzmann weight" for a system of hard spheres of diameter a and centers in the positions $\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N$:

$$\Psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N) = \frac{1}{\sqrt{Z_N^{(c)}}} \ F_N(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N) \tag{106}$$

where

$$F_N(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_N) = \begin{cases} 1 & |\boldsymbol{r}_i - \boldsymbol{r}_j| > a, \ \forall i \neq j \\ 0 & \text{otherwise} \end{cases} \tag{107}$$

22.1

Show that $Z_N^{(c)}$ is the configurational partition function (namely the partition function for the position space only) of the hard sphere gas in the distinguishable-particle case (or $N! \ Z_N^{(c)}$ for the indistinguishable-particle case).

22.2

Justify that, for $|\boldsymbol{r}-\boldsymbol{r}'|>a$:

$$F_N(\boldsymbol{r},\boldsymbol{r}_2,...,\boldsymbol{r}_N)\ F_N(\boldsymbol{r}',\boldsymbol{r}_2,...,\boldsymbol{r}_N)=F_{N+1}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}_2,...,\boldsymbol{r}_N) \tag{108}$$

22.3

The one-body density matrix at $T=0$ takes the form

$$g^{(1)}(\boldsymbol{r},\boldsymbol{r}')=N\int d^3r_2...d^3r_N\Psi_0(\boldsymbol{r},\boldsymbol{r}_2,...,\boldsymbol{r}_N)\Psi_0(\boldsymbol{r}',\boldsymbol{r}_2,...,\boldsymbol{r}_N). \tag{109}$$

Justify that, for $|\boldsymbol{r}-\boldsymbol{r}'|>a$

$$g^{(1)}(\boldsymbol{r},\boldsymbol{r}')=\frac{Z^{(c)}_{N+1}}{Z^{(c)}_N}\frac{1}{N+1}\ \rho_2(\boldsymbol{r},\boldsymbol{r}') \tag{110}$$

where $\rho_2(\boldsymbol{r},\boldsymbol{r}')$ is the so-called pair correlation function, namely $\rho_2(\boldsymbol{r},\boldsymbol{r}')\ d^3r\ d^3r'$ gives the probability of finding any two spheres (out of $N+1$) with centers in the infinitesimal volumes d^3r and d^3r' centered around $\boldsymbol{r}$ and $\boldsymbol{r}'$ respectively.

22.4

Justify that, in the limit $|\boldsymbol{r}-\boldsymbol{r}'|\to\infty$, $\rho_2(\boldsymbol{r},\boldsymbol{r}')\to(N/V)^2$ (where $N\gg 1$). Reminding yourself of the relationship between the condensate density n_0 and the one-body density matrix, show that

$$n_0=z\left(\frac{N}{V}\right)^2 \tag{111}$$

where $z=(Z^{(c)}_{N+1}/Z^{(c)}_N)\ N!/(N+1)!$.

22.5

We introduce the function

$$f(v_N)=\frac{1}{N}\log\frac{Z^{(c)}_N}{N!\ v_0^N}\qquad (N\to\infty) \tag{112}$$

where $v_N=V/N$ and v_0 is a reference volume. What is its physical meaning ? Show that

$$\frac{1}{N+1}\log\frac{Z^{(c)}_{N+1}}{(N+1)!\ v_0^{N+1}}\approx f(v_N)-\frac{v_N}{N}\frac{\partial f}{\partial v}(v_N) \tag{113}$$

and consequently in the thermodynamic limit ($v_N\to v$ independent of N)

$$\log(z/v_0)\approx f(v)-v\frac{\partial f}{\partial v}(v)\ . \tag{114}$$

22.6

We now consider the hard-sphere gas with both kinetic and configurational terms of the partition function. The equation of state of a classical interacting gas is given by

$$P=k_BT\left(\frac{N}{V}+\frac{\partial}{\partial V}\log\frac{Z^{(c)}_N}{V^N}\right) \tag{115}$$

How do we obtain the ideal gas limit ?

The second term on the right-hand side, stemming from interactions, can be calculated via the so-called virial expansion when the range of the interaction potential is small compared to the interparticle distance (in our case $na^3 \ll 1$, where $n = N/V$)

$$P = k_B T \left[\frac{N}{V} + B_2 \left(\frac{N}{V} \right)^2 + B_3 \left(\frac{N}{V} \right)^3 + ... \right] \tag{116}$$

For the hard-sphere gas, this expansion gives

$$B_2 = \frac{2\pi}{3} a^3 \tag{117}$$

From Eqs. (**??**) and (**??**) find a differential equation for $Z_N^{(c)}$ and hence for $f(v)$. Show that it is solved by

$$f(v) = \log v - \frac{2\pi}{3} \frac{a^3}{v} + 1 \tag{118}$$

22.7

Calculate z as a function of v and a. Using the data for ^{4}He, $a = 2.56$ Å and $v = 46.2$ Å^3, calculate the condensate fraction $N_0/N = n_0 V/N$. How does it compare with the value measured in ^{4}He by neutron scattering ($N_0/N = 6 - 8$ %) ?

TD7 : Condensate in a rotating annulus

In this exercise we shall explore the properties of a condensate put under rotation in a non-simply connected geometry (namely in a container with a hole). The simplest example is a so-called *annulus*, namely a circular container with very small thickness compared to its radius, as shown in Fig. **??**(a). The annulus is set into rotation at angular velocity Ω perpendicular to the plane.

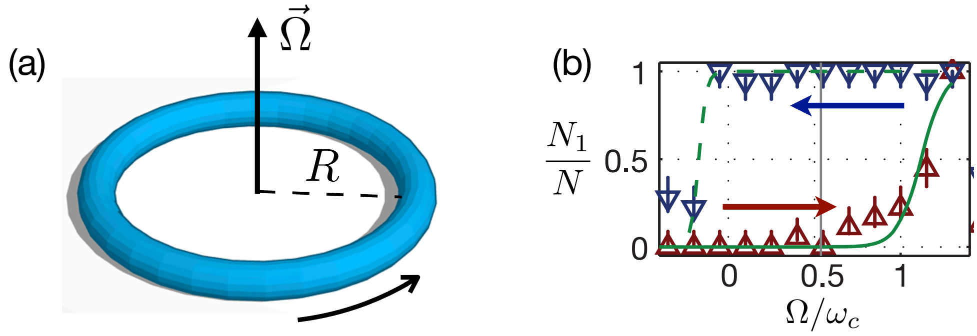


FIGURE 5 – (a) Rotating annulus ; (b) Experimental data of the fraction of atoms N_1/N with angular momentum $m = 1$ (from S. Eckel et al., Nature 506, 200 (2014)). Red (upward) triangles correspond to the recorded fraction when increasing the rotation frequency Ω from negative to positive ; blue (downward) triangles correspond to the fraction recorded when decreasing the frequency back to negative.

23 Single particle in a rotating annulus

The Hamiltonian of a single quantum particle in a rotating annulus in the laboratory frame has the form

$$\mathcal{H}_{\rm lab} = \frac{\boldsymbol{p}^2}{2M} + W(\boldsymbol{r}, t) \tag{119}$$

where W is the (time-dependent) confining potential of the annulus. Its time dependence comes from the fact that the container is not perfectly cylindrically symmetric. Yet, in order to investigate the equilibrium physics of this problem, we have to move to the *rotating frame*, co-rotating with the annulus, in which the potential becomes time independent, $U(\boldsymbol{r})$ – and we shall neglect its imperfect cylindrical symmetry in the following. The full Hamiltonian in the rotating frame reads

$$\mathcal{H} = \frac{\boldsymbol{p}^2}{2M} + U(\boldsymbol{r}) - \Omega L^z \tag{120}$$

where $L^z = xp_y - yp_x$ is the angular momentum along the axis of rotation.

23.1

Show that the Hamiltonian in the rotating frame can be cast in the form

$$\mathcal{H} = \frac{(\boldsymbol{p} + q\boldsymbol{A})^2}{2M} + U(\boldsymbol{r}) + U_{\rm centr}(\boldsymbol{r}) \tag{121}$$

where q is a fictitious charge (which can be set to 1), $\boldsymbol{A}$ is a fictitious vector potential (associated with the Coriolis force), and $U_{\rm centr}$ is the centrifugal potential (to be specified).

23.2

Show that the fictitious magnetic field associated with $\boldsymbol{A}$ reads $\boldsymbol{B} = (2M\Omega/q)\boldsymbol{e}_z$.

23.3

We recall the expression of the angular momentum, of the gradient and of the Laplacian in cylindrical coordinates

$$L^z = -i\hbar\frac{\partial}{\partial\phi} \qquad \boldsymbol{\nabla} = \frac{\partial}{\partial r}\,\boldsymbol{e}_r + \frac{1}{r}\frac{\partial}{\partial\phi}\,\boldsymbol{e}_\phi + \frac{\partial}{\partial z}\,\boldsymbol{e}_z \qquad \nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}\ . \tag{122}$$

Show that the Hamiltonian can be written as $\mathcal{H} = \mathcal{H}_{r,z} + \mathcal{H}_{r,\phi}$, where

$$\begin{aligned} \mathcal{H}_{r,z} &= -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}\right) + U(r,z) + U_{\mathrm{centr}}(r) \\ \mathcal{H}_{r,\phi} &= \frac{\hbar^2}{2Mr^2}\left(-i\frac{\partial}{\partial\phi} - \frac{\Omega M r^2}{\hbar}\right)^2\ . \end{aligned} \tag{123}$$

23.4

We will solve the Schrödinger's equation by separation of variables, namely in the form $\psi(r,z,\phi) \approx \chi(r,z)\Phi(\phi)$. We ask that $\mathcal{H}_{r,z}\ \chi = E_\perp\ \chi$. The "annulus condition" amounts to the fact that, in spite of the centrifugal potential, $U(r,z)$ confines a particle so tightly that $\chi(r,z) \sim \sqrt{\delta(r-R)}$ in the ground state of motion along r and z.
Conclude that Φ satisfies the equation

$$\frac{\hbar^2}{2MR^2}\left(-i\frac{\partial}{\partial\phi} - \frac{\Omega}{\omega_c}\right)^2 \Phi(\phi) = (E - E_\perp)\,\Phi(\phi) \tag{124}$$

where $\omega_c = \hbar/(MR^2)$.

23.5

The solution for the above Schrödinger's equation has the form $\Phi(\phi) = e^{im\phi}/\sqrt{2\pi}$ with $m \in \mathbb{Z}$. Calculate the corresponding eigenvalue $E_{||}(m;\Omega) = E - E_\perp$. Plot the eigenvalues as a function of Ω for various values of m, and establish the m value which corresponds to the ground state.

23.6

The tangential velocity associated with the $\Phi(\phi) = |\Phi|e^{i\varphi(\phi)}$ wavefunction is $\boldsymbol{v}_s = \frac{\hbar}{M}\boldsymbol{\nabla}\varphi$. Show that the circulation κ of the velocity along the annulus is quantized in units of h/M. Plot the ground-state tangential velocity and the corresponding angular velocity as a function of Ω. Does it ever happen that the particle rotates *faster* than the ring ?

24 Many-body problem : metastable superflow

We now move to the many-body problem for a system of N identical bosons interacting with a contact repulsive potential ($g > 0$), with Hamiltonian

$$\hat{\mathcal{H}} = \int d^3r\ \hat{\psi}^\dagger(\boldsymbol{r})\ [\mathcal{H}_{rz} + \mathcal{H}_{r\phi}]\ \hat{\psi}(\boldsymbol{r}) + \frac{g}{2}\int d^3r\ \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\ . \tag{125}$$

We suppose that the particles are all in the ground state corresponding to the motion along r and z, so that

$$\hat{\psi}(\boldsymbol{r}) \approx \chi(r,z)\sum_m \frac{e^{im\phi}}{\sqrt{2\pi}}\ \hat{a}_m\ . \tag{126}$$

24.1

Show that the Hamiltonian written in terms of the $\hat{a}_m, \hat{a}_m^\dagger$ operators takes the form

$$\hat{\mathcal{H}} = E_\perp N + \sum_m \frac{\hbar\omega_c}{2}(m - \Omega/\omega_c)^2 \hat{a}_m^\dagger \hat{a}_m + \frac{U}{2} \sum_{m,m',p} a_{m+p}^\dagger a_{m'-p}^\dagger \hat{a}_{m'} \hat{a}_m \tag{127}$$

where U is a coefficient to be determined.

24.2

Assuming that $U \ll \hbar\omega_c$, we consider that the interaction can only connect two angular momentum states $m, m+1$ which are brought into degeneracy by tuning Ω. Without loss of generality we choose $m = 0, 1$. By restricting all sums over m to these two values, show that the Hamiltonian reduces to a function of the occupation numbers $\hat{n}_0 = \hat{a}_0^\dagger \hat{a}_0$ and $\hat{n}_1 = \hat{a}_1^\dagger \hat{a}_1$.

24.3

The Hamiltonian eigenstates are therefore Fock states of the kind $|N_0, N_1\rangle$ (where all other m states are empty). In the following we set $E_\perp = 0$. Show that the corresponding eigenvalue takes the form $E = E_{\text{kin}} + E_{\text{pot}}$ with

$$E_{\text{kin}} = N\frac{\hbar\omega_c}{2}\left(1 - \frac{2\Omega}{\omega_c}\right) f_1 + C \qquad E_{\text{pot}} = UN^2(1 - f_1)f_1 + C' \tag{128}$$

where $f_1 = N_1/N$ is the fraction of particles in the $m = 1$ state, and C and C' are two constants to be determined.

24.4

Plot $E = E(f_1; \Omega)$ as a function of f_1 for $\Omega < \omega_c/2$, $\Omega = \omega_c/2$ and $\Omega > \omega_c/2$. What happens to the equilibrium value of f_1 upon crossing the $\omega_c/2$ angular velocity ?

24.5

Imagine now an experiment in which the gas is first prepared in a perfect condensate with $m = 0$ and $\Omega = 0$, and then the annulus is set gradually into rotation. What happens to f_1 if Ω is not varied infinitely slowly ? Similarly you can imagine to prepare the gas in the ground state at $\Omega = \omega_c$, and then slow down gradually the rotation. The results of such an experiment (done on ultracold Rb atoms in an optical ring potential) are shown in Fig. **??**(b). Deduce that the motion of the gas can exhibit an effective *decoupling* with respect to the walls of its container, in the form of a persistent state of rest, or of a persistent superflow.

TD7bis : Fermions – coherence properties and pairing

25 Quantum coherence in a fermion gas

We here consider the correlation function of first and second order in a fermion gas.

25.1

Considering an ideal spinless Fermi gas in $d = 3$, we want to calculate the one-body density matrix (or first-order correlation function)

$$g^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = \langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}')\rangle \quad . \tag{129}$$

Using the momentum representation of the field operators

$$\hat{\psi}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \hat{c}_{\boldsymbol{k}} \tag{130}$$

and considering that, at $T = 0$, the Fermi gas occupies a Fermi sphere of radius k_F in momentum space, show that $g^{(1)}(\boldsymbol{r}, \boldsymbol{r}')$ reads

$$g^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = \frac{1}{2\pi^2 R^2}\left[\frac{\sin(k_F R)}{R} - k_F\cos(k_F R)\right] \tag{131}$$

where $R = |\boldsymbol{r} - \boldsymbol{r}'|$. Sketch the behavior of $g^{(1)}$ for $R \to \infty$ and comment on the physical meaning of this limit. Taking the opposite limit $g^{(1)}(R \to 0)$ show that $k_F = (6\pi^2 n)^{1/3}$ where $n = N/V$ is the density of the spinless Fermi gas.

25.2

We consider a generic $S = 1/2$ Fermi gas, and we introduce the *pair correlation function*

$$g^{(2)}(\boldsymbol{r}, \boldsymbol{r}') = V\langle \hat{\psi}^\dagger_\downarrow(\boldsymbol{r})\hat{\psi}^\dagger_\uparrow(\boldsymbol{r})\hat{\psi}_\uparrow(\boldsymbol{r}')\hat{\psi}_\downarrow(\boldsymbol{r}')\rangle \quad . \tag{132}$$

Using the momentum representation of the field operators, and considering a system in which the momentum is conserved, show that, for $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$

$$g^{(2)}(\boldsymbol{r}, \boldsymbol{r}') \approx \frac{1}{V}\sum_{\boldsymbol{k}} \langle \hat{\mathcal{S}}^\dagger_{\boldsymbol{k}} \hat{\mathcal{S}}_{\boldsymbol{k}}\rangle \; + \; \text{(rapidly oscillating terms)} \tag{133}$$

where we have introduced the operator

$$\hat{\mathcal{S}}^\dagger_{\boldsymbol{k}} = \frac{1}{\sqrt{2}}\left(\hat{c}^\dagger_{\boldsymbol{k}\uparrow}\hat{c}^\dagger_{-\boldsymbol{k}\downarrow} - \hat{c}^\dagger_{\boldsymbol{k}\downarrow}\hat{c}^\dagger_{-\boldsymbol{k}\uparrow}\right) \quad . \tag{134}$$

25.3

Consider the two-particle wavefunction $|\psi\rangle = \hat{\mathcal{S}}^\dagger_{\boldsymbol{k}}|0\rangle$. Remembering that, for fermions

$$\psi(\boldsymbol{r}, \sigma; \boldsymbol{r}', \sigma) = \frac{1}{\sqrt{2}}\left(\langle \boldsymbol{r}, \sigma; \boldsymbol{r}', \sigma'| - \langle \boldsymbol{r}', \sigma'; \boldsymbol{r}, \sigma|\right)|\psi\rangle \tag{135}$$

show that $\psi(\boldsymbol{r}, \sigma; \boldsymbol{r}', \sigma)$ describes two particles with opposite momenta and with spins forming a singlet state $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ (Cooper pair). Conclude on the relationship between the pair correlation function and the density of Cooper pairs.

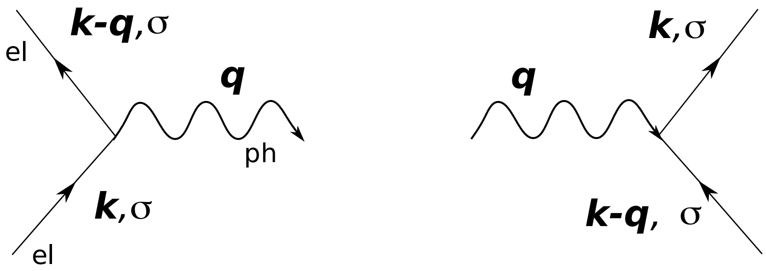


FIGURE 6 – Emission (left) and absorption (right) of a phonon by an electron interacting with the ion lattice.

25.4

We return to the ideal Fermi gas, this time with spin. Show that, for this system

$$g^{(2)}(\boldsymbol{r},\boldsymbol{r}') = V g^{(1)}_{\uparrow}(\boldsymbol{r},\boldsymbol{r}') g^{(1)}_{\downarrow}(\boldsymbol{r},\boldsymbol{r}') \quad . \tag{136}$$

How does this function decay for $|\boldsymbol{r}-\boldsymbol{r}'| \to \infty$? Conclude on the density of pairs in the ideal Fermi gas.

26 Quantum-mechanical description of electron-electron interactions mediated by phonons

Consider the electron gas in a metal. A minimal model describing both the (non-interacting) electrons, the phonons of the ion lattice, and their interaction, is the following Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\rm ph} + \hat{\mathcal{H}}_{\rm el} + \hat{\mathcal{H}}_{\rm el-ph} \tag{137}$$

where

$$\begin{aligned} \hat{\mathcal{H}}_{\rm ph} &= \sum_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}} \; \hat{b}^\dagger_{\boldsymbol{q}} \hat{b}_{\boldsymbol{q}} \\ \hat{\mathcal{H}}_{\rm el} &= \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \; \hat{c}^\dagger_{\boldsymbol{k},\sigma} \hat{c}_{\boldsymbol{k},\sigma} \\ \hat{\mathcal{H}}_{\rm el-ph} &= \gamma \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \left(\hat{b}^\dagger_{\boldsymbol{q}} \; \hat{c}^\dagger_{\boldsymbol{k}-\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma} + \text{h.c.} \right) \end{aligned} \tag{138}$$

The last term describes the elementary quantum mechanical processes of interaction between an electron and the ion lattice : an electron emits or aborbs a phonon from the lattice, thereby losing/gaining a momentum $\hbar\boldsymbol{q}$. A pictorial way to represent this process is the one shown in Fig. ??.
We imagine that the initial configuration of the system consists of two electrons in the anti-symmetrized state $|\psi(0)\rangle = |\boldsymbol{k},\sigma;\boldsymbol{k}',\sigma'\rangle = \hat{c}^\dagger_{\boldsymbol{k},\sigma}\hat{c}^\dagger_{\boldsymbol{k}',\sigma'}|0\rangle$, moving in the vacuum of phonons. This state is clearly an eigenstate of $\hat{\mathcal{H}}_{\rm ph} + \hat{\mathcal{H}}_{\rm el}$. Treating $\hat{\mathcal{H}}_{\rm el-ph}$ as a perturbation, it introduces a finite matrix element between the initial state and a state $|\psi(\boldsymbol{q})\rangle = |\boldsymbol{k}-\boldsymbol{q},\sigma;\boldsymbol{k}'+\boldsymbol{q},\sigma'\rangle$. Within second-order perturbation theory, this matrix element reads

$$\langle\psi(\boldsymbol{q})|\hat{\mathcal{H}}|\psi(0)\rangle \approx \frac{1}{2}\sum_n \left(\frac{1}{E_0-E_n} + \frac{1}{E_{\boldsymbol{q}}-E_n}\right) \langle\psi(\boldsymbol{q})|\hat{\mathcal{H}}_{\rm el-ph}|\psi_n\rangle\langle\psi_n|\hat{\mathcal{H}}_{\rm el-ph}|\psi(0)\rangle \tag{139}$$

where $|\psi_n\rangle$ are intermediate eigenstates of $\hat{\mathcal{H}}_{\rm ph} + \hat{\mathcal{H}}_{\rm el}$ different from (and non-degenerate with) $|\psi(\boldsymbol{q})\rangle$ and $|\psi(0)\rangle$. Moreover $E_0 = \epsilon_{\boldsymbol{k}} + \epsilon_{\boldsymbol{k}'}$ and $E_{\boldsymbol{q}} = \epsilon_{\boldsymbol{k}-\boldsymbol{q}} + \epsilon_{\boldsymbol{k}'+\boldsymbol{q}}$.

26.1

Identify the intermediate states $|\psi_n\rangle$ leading to non vanishing contributions in the sum of Eq. (**??**) , and calculate them. Show that

$$\langle\psi(\boldsymbol{q})|\hat{\mathcal{H}}_{\mathrm{el-ph}}|\psi(0)\rangle = -\gamma^2\left[\frac{\hbar\omega_{\boldsymbol{q}}}{(\hbar\omega_{\boldsymbol{q}})^2-(\epsilon_{\boldsymbol{k}-\boldsymbol{q}}-\epsilon_{\boldsymbol{k}})^2}+\frac{\hbar\omega_{\boldsymbol{q}}}{(\hbar\omega_{\boldsymbol{q}})^2-(\epsilon_{\boldsymbol{k}'+\boldsymbol{q}}-\epsilon_{\boldsymbol{k}'})^2}\right] \tag{140}$$

Can you relate this matrix element to the process of exchange of (virtual) phonons between the electrons? Why are these phonons *virtual* and not real?

26.2

Write the reduced 2×2 Hamiltonian on the Hilbert space spanned by $|\psi(\boldsymbol{q})\rangle$ and $|\psi(0)\rangle$ (namely the matrix $\langle\psi|\mathcal{H}|\psi'\rangle$ where $|\psi\rangle$, $|\psi'\rangle = |\psi(\boldsymbol{q})\rangle$, $|\psi(0)\rangle$). Discuss why the maximum "mixing" between these two states is achieved when $\boldsymbol{q}=2\boldsymbol{k}$ and $\boldsymbol{k}'=-\boldsymbol{k}$. Show that in this case the matrix element, Eq. (**??**), takes a negative value $-\Gamma$, with $\Gamma>0$ to be determined.

26.3

Diagonalising the reduced Hamiltonian described above, show that the minimum energy state in this subspace is

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}\left(\hat{c}^\dagger_{\boldsymbol{k},\sigma}\hat{c}^\dagger_{-\boldsymbol{k},\sigma'}-\hat{c}^\dagger_{\boldsymbol{k},\sigma'}\hat{c}^\dagger_{-\boldsymbol{k},\sigma}\right)|0\rangle \tag{141}$$

having energy $2\epsilon_{\boldsymbol{k}}-\Gamma$. For what values of σ and σ' is this state non-zero? Comparing with the result of Exercise 1.3, what can you conclude on the nature of the $|\psi_0\rangle$ state? In conclusion, what is the effect of the exchange of phonons between two electrons? Based on the results of Exercise 1.2, how do you expect it to affect the long-distance behavior of the pair correlation function $g^{(2)}$?

TD8 : Anderson's pseudo-spin model and BCS variational wavefunction

In this TD we will explore a very insightful approach to the BCS Hamiltonian provided by P. W. Anderson (1958). Recasting the BCS Hamiltonian in terms of pseudo-spin variables, we will be able to write down the ground state of BCS theory in a very transparent and suggestive way.
NOTE : the angle $\vartheta_{\boldsymbol{k}}$ that appears in the following is not the same as the angle $\theta_{\boldsymbol{k}}$ discussed in the lectures on BCS theory. We shall establish the relationship between the two later.

27 Pair operators and spin operators

Consider the pair operators

$$\hat{b}_{\boldsymbol{k}} = \hat{c}_{-\boldsymbol{k}\downarrow}\hat{c}_{\boldsymbol{k}\uparrow} \qquad \hat{b}^{\dagger}_{\boldsymbol{k}} = \hat{c}^{\dagger}_{\boldsymbol{k}\uparrow}\hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow} \tag{142}$$

27.1

Show that

$$\left[\hat{b}_{\boldsymbol{k}}, \hat{b}_{\boldsymbol{q}}\right] = \left[\hat{b}^{\dagger}_{\boldsymbol{k}}, \hat{b}^{\dagger}_{\boldsymbol{q}}\right] = 0 \tag{143}$$

$$\left[\hat{b}_{\boldsymbol{k}}, \hat{b}^{\dagger}_{\boldsymbol{q}}\right] = (1 - n_{\boldsymbol{k},\uparrow} - n_{-\boldsymbol{k},\downarrow})\,\delta_{\boldsymbol{q},\boldsymbol{k}} \tag{144}$$

Moreover, justify that $(b^{\dagger}_{\boldsymbol{k}})^2 = (b_{\boldsymbol{k}})^2 = 0$.

27.2

Introducing the operators (Anderson's pseudospins)

$$\begin{aligned} \hat{S}^z_{\boldsymbol{k}} &= \frac{1}{2}\left(\hat{n}_{\boldsymbol{k},\uparrow} + \hat{n}_{-\boldsymbol{k},\downarrow} - 1\right) \\ \hat{S}^+_{\boldsymbol{k}} &= \hat{b}^{\dagger}_{\boldsymbol{k}} \\ \hat{S}^-_{\boldsymbol{k}} &= \hat{b}_{\boldsymbol{k}} \end{aligned} \tag{145}$$

show that they satisfy the commutation relations of angular momentum

$$\left[\hat{S}^+_{\boldsymbol{k}}, \hat{S}^-_{\boldsymbol{k}}\right] = 2\hat{S}^z_{\boldsymbol{k}} \qquad \left[\hat{S}^+_{\boldsymbol{k}}, \hat{S}^z_{\boldsymbol{k}}\right] = -\hat{S}^+_{\boldsymbol{k}} \tag{146}$$

Given that $(\hat{S}^+_{\boldsymbol{k}})^2 = (\hat{S}^-_{\boldsymbol{k}})^2 = 0$, what is the spin length S ?

28 BCS Hamiltonian as a spin Hamiltonian

The BCS Hamiltonian for (quasi-)electrons interacting via an effective phonon-mediated interaction reads

$$\hat{\mathcal{H}} - \mu\hat{N} = \sum_{\boldsymbol{k}} (\epsilon_{\boldsymbol{k}} - \mu)\,(\hat{n}_{\boldsymbol{k},\uparrow} + \hat{n}_{\boldsymbol{k},\downarrow}) - \frac{V_0}{\mathcal{V}} {\sum_{\boldsymbol{k},\boldsymbol{q}}}' \hat{b}^{\dagger}_{\boldsymbol{k}}\hat{b}_{\boldsymbol{q}} \quad . \tag{147}$$

Here $\mathcal{V}$ is the volume, V_0 is the strength of the interaction, and the sum ${\sum_{\boldsymbol{k},\boldsymbol{q}}}'$ runs over momenta $\boldsymbol{k}$ and $\boldsymbol{q}$ such that $|\epsilon_{\boldsymbol{k}(\boldsymbol{q})} - \mu| \leq \epsilon_c$, where $\epsilon_c \approx \hbar\omega_D$ is the characteristic energy cutoff of the interaction.

28.1

Rewrite the above Hamiltonian in terms of the pseudo-spin operators. You should find

$$\hat{\mathcal{H}} - \mu\hat{N} = \sum_{\boldsymbol{k}} \left[2\left(\epsilon_{\boldsymbol{k}} - \mu\right) - \frac{V_0}{\mathcal{V}}\ \vartheta\left(\epsilon_c - |\epsilon_{\boldsymbol{k}} - \mu|\right)\right] \hat{S}^z_{\boldsymbol{k}} - \frac{V_0}{\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{q}}{}' \left(\hat{S}^x_{\boldsymbol{k}}\hat{S}^x_{\boldsymbol{q}} + \hat{S}^y_{\boldsymbol{k}}\hat{S}^y_{\boldsymbol{q}}\right) + \text{const.} \tag{148}$$

It might be useful to remember the following relationships

$$\hat{S}^+_{\boldsymbol{k}}\hat{S}^-_{\boldsymbol{k}} = \frac{1}{2} + \hat{S}^z_{\boldsymbol{k}} \qquad \frac{1}{2}\left(\hat{S}^+_{\boldsymbol{k}}\hat{S}^-_{\boldsymbol{q}} + \hat{S}^+_{\boldsymbol{q}}\hat{S}^-_{\boldsymbol{k}}\right) = \hat{S}^x_{\boldsymbol{k}}\hat{S}^x_{\boldsymbol{q}} + \hat{S}^y_{\boldsymbol{k}}\hat{S}^y_{\boldsymbol{q}} \quad . \tag{149}$$

Now, think of $\boldsymbol{k}$-space as a lattice (it is discretized after all, due to the boundary conditions), and put a $S = 1/2$ (pseudo-)spin on each lattice site. The above Hamiltonian effectively describes a system of interacting spins on a lattice. Taking the spin at lattice site $\boldsymbol{k}$, which are the sites that this spin is interacting with? And what is the value of the local magnetic field?

28.2

We take for the moment $V_0 = 0$. Write down the ground state for each pseudo-spin $\hat{S}_{\boldsymbol{k}}$. If you report the $\boldsymbol{k}$ points on the energy axis $\epsilon_{\boldsymbol{k}}$ (a simply sketch is sufficient) together with the associated pseudo-spin, can you find a "domain wall" at a given energy in the spin configuration? And can you anticipate qualitatively what happens when the interaction is turned on?

29 BCS variational wavefunction

We now look for the ground state of the interacting system ($V_0 \neq 0$) in a *factorized* form, namely in the form

$$|\Psi_0\rangle = \prod_{\boldsymbol{k}} |\vartheta_{\boldsymbol{k}}, \phi_{\boldsymbol{k}}\rangle \tag{150}$$

where

$$|\vartheta, \phi\rangle = \cos(\vartheta/2)\ |\uparrow\rangle + \sin(\vartheta/2)\ e^{i\phi}\ |\downarrow\rangle \tag{151}$$

29.1

Show that the above wavefunction is equivalent to the so-called BCS wavefunction

$$|\Psi_0\rangle = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}} + v_{\boldsymbol{k}}\ \hat{b}^\dagger_{\boldsymbol{k}}\right)|0\rangle \tag{152}$$

where the coefficients $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ are to be identified. (Suggestion : write the vacuum $|0\rangle$ in terms of the pseudo-spin states).

29.2

Show that the expectation value of the spin operator $\hat{\boldsymbol{S}}$ on the $|\vartheta, \phi\rangle$ state behaves like a classical spin of length $S = 1/2$:

$$\langle\vartheta, \phi|\hat{\boldsymbol{S}}|\vartheta, \phi\rangle = \frac{1}{2}\left(\cos\phi\sin\vartheta, \sin\phi\sin\vartheta, \cos\vartheta\right) \tag{153}$$

and, moreover

$$\langle\vartheta_{\boldsymbol{k}}, \phi_{\boldsymbol{k}}|\langle\vartheta_{\boldsymbol{q}}, \phi_{\boldsymbol{q}}|\left(\hat{S}^x_{\boldsymbol{k}}\hat{S}^x_{\boldsymbol{q}} + \hat{S}^y_{\boldsymbol{k}}\hat{S}^y_{\boldsymbol{q}}\right)|\vartheta_{\boldsymbol{k}}, \phi_{\boldsymbol{k}}\rangle|\vartheta_{\boldsymbol{q}}, \phi_{\boldsymbol{q}}\rangle = \frac{1}{4}\cos\left(\phi_{\boldsymbol{k}} - \phi_{\boldsymbol{q}}\right)\sin\vartheta_{\boldsymbol{k}}\sin\vartheta_{\boldsymbol{q}} \tag{154}$$

Show that the variational energy takes the form

$$\langle\Psi_0|\hat{\mathcal{H}} - \mu\hat{N}|\Psi_0\rangle = \sum_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} - \mu - \frac{V_0}{2\mathcal{V}}\ \vartheta\left(\epsilon_c - |\epsilon_{\boldsymbol{k}} - \mu|\right)\right]\cos\vartheta_{\boldsymbol{k}} \ - \ \frac{V_0}{4\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{q}}{}' \cos\left(\phi_{\boldsymbol{k}} - \phi_{\boldsymbol{q}}\right)\sin\vartheta_{\boldsymbol{k}}\sin\vartheta_{\boldsymbol{q}} \tag{155}$$

Given that $V_0 > 0$ and $\vartheta_{\boldsymbol{k}} \in [0, \pi]$, what value of the $\phi_{\boldsymbol{k}}$ angles minimizes the energy?

29.3

Minimize the variational energy with respect to $\vartheta_{\boldsymbol{k}}$ for $|\epsilon_{\boldsymbol{k}} - \mu| < \epsilon_c$, to find the condition

$$\left(\epsilon_{\boldsymbol{k}} - \mu - \frac{V_0}{2\mathcal{V}}\right) \sin\vartheta_{\boldsymbol{k}} = -\frac{V_0}{2\mathcal{V}} \sum_{\boldsymbol{q}\neq\boldsymbol{k}}{}' \sin\vartheta_{\boldsymbol{q}} \cos\vartheta_{\boldsymbol{k}} \tag{156}$$

This condition defines a set of coupled equations.
Making an error of order $\mathcal{O}(1/\mathcal{V})$, we can neglect the term $V_0/(2\mathcal{V})$ on the left-hand side and the add the term with $\boldsymbol{q} = \boldsymbol{k}$ in the sum on the right-hand side.
Introducing then the symbol

$$\Delta = \frac{V_0}{2\mathcal{V}} \sum_{\boldsymbol{q}}{}' \sin\vartheta_{\boldsymbol{q}} \tag{157}$$

rewrite Eq. (**??**) in terms of Δ, $\epsilon_{\boldsymbol{k}}$, μ and $\vartheta_{\boldsymbol{k}}$.

29.4

Solve for $\vartheta_{\boldsymbol{k}}$, to find

$$\sin\vartheta_{\boldsymbol{k}} = \frac{\Delta}{E_{\boldsymbol{k}}} \qquad \cos\vartheta_{\boldsymbol{k}} = \frac{\mu - \epsilon_{\boldsymbol{k}}}{E_{\boldsymbol{k}}} \qquad E_{\boldsymbol{k}} = \sqrt{\Delta^2 + (\epsilon_{\boldsymbol{k}} - \mu)^2} \tag{158}$$

What is the pseudo-spin orientation at the Fermi energy $\epsilon_F = \mu$? Draw schematically how the pseudo-spin orientation evolve when the energy goes from $\mu - \epsilon_c$ to $\mu + \epsilon_c$.

29.5

From Eq. (**??**) recover the (implicit) gap equation for $|\Delta|$ as seen in the lecture.

30 Average particle number

The BCS wavefunction, Eq. (**??**), does not contain a well defined particle number. In particular, $|\Psi_0\rangle$ contains all possible *even* particle numbers from 0 to ∞. But let us have a look at how well defined the *average* particle number is

30.1

Express the average particle number

$$\langle \hat{N} \rangle = \sum_{\boldsymbol{k}} \langle \hat{n}_{\boldsymbol{k},\uparrow} + \hat{n}_{\boldsymbol{k},\downarrow} \rangle \tag{159}$$

and the average square number

$$\langle \hat{N}^2 \rangle = \sum_{\boldsymbol{k},\boldsymbol{q}} \langle (\hat{n}_{\boldsymbol{k},\uparrow} + \hat{n}_{\boldsymbol{k},\downarrow}) (\hat{n}_{\boldsymbol{q},\uparrow} + \hat{n}_{\boldsymbol{q},\downarrow}) \rangle \tag{160}$$

in terms of the $\vartheta_{\boldsymbol{k}}$ angles.

30.2

Show that

$$\langle \delta^2 \hat{N} \rangle = \sum_{\boldsymbol{k}} \left(1 - \langle \cos\vartheta_{\boldsymbol{k}} \rangle^2\right) \sim \mathcal{O}(N) \tag{161}$$

How can one conclude that the sum is $\mathcal{O}(N)$? Which $\boldsymbol{k}$ states are contributing to it ?

30.3

Conclude on the importance of the relative particle-number fluctuations.

31 Angle $\vartheta_{\boldsymbol{k}}$ vs. angle $\theta_{\boldsymbol{k}}$

Consider the angle $\theta_{\boldsymbol{k}}$ given in the lectures on BCS theory (such that $u_{\boldsymbol{k}} = \cos(\theta_{\boldsymbol{k}}/2)$, $v_{\boldsymbol{k}} = \sin(\theta_{\boldsymbol{k}}/2)$) : what is the relationship with the angle $\vartheta_{\boldsymbol{k}}$ introduced in this exercise ?

TD9 : Superconductors in a magnetic field

Useful formulae

— Gradient in cylindrical coordinates (on the cylinder surface) :

$$\nabla = \frac{1}{R}\frac{\partial}{\partial\theta}\hat{e}_\theta + \frac{\partial}{\partial z}\hat{e}_z. \tag{162}$$

— Closest integer n to a real number a

$$n = \mathrm{int}(a + \mathrm{sign}(a)\ 1/2). \tag{163}$$

— For a closed path γ encircling the surface S_γ

$$\oint_\gamma \boldsymbol{A}\cdot d\boldsymbol{l} = \int_{S_\gamma} \boldsymbol{B}\cdot\hat{n}\ dS_\gamma = \Phi_\gamma(\boldsymbol{B}) = \text{flux of } \boldsymbol{B} \text{ through } S_\gamma \tag{164}$$

32 Flux quantization in a superconducting cylinder

In this exercise we wish to describe the fundamental phenomenon of quantization of the magnetic flux which threads a superconducting cylinder. For this purpose, we will start with a description of the problem of a single electron confined in a cylinder of radius R, height L, immersed in a uniform magnetic field $\boldsymbol{B} = (0, 0, B)$ parallel to the axis of the cylinder (see Fig. **??**). We will assume periodic boundary conditions along the z axis. The cross section of the cylinder forms a ring, whose thickness will be neglected for the moment.

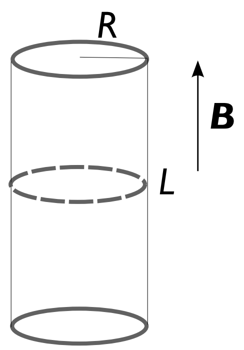


FIGURE 7 –

The Hamiltonian of an electron in a magnetic field reads

$$\mathcal{H} = \frac{(-i\hbar\nabla + e\boldsymbol{A})^2}{2m} \tag{165}$$

We take for the vector potential the symmetric gauge $\boldsymbol{A} = \frac{B}{2}(-y, x, 0)$. Passing to cylindrical coordinates (r, θ, z), the vector potential on the cylindrical surface reads $\boldsymbol{A} = (BR/2)\hat{e}_\theta$.

32.1

Justify that the eigenvectors of the Hamiltonian have the form

$$\psi_{n,k_z}(\theta, z) = \mathcal{N} \exp(in\theta) \exp(ik_z z) \tag{166}$$

where $\mathcal{N}$ is a normalization constant to be determined, and n is an *integer*.
Show that the eigenvalues of the Hamiltonian take the form

$$E_{n,k_z} = \frac{\hbar^2}{2mR^2} \left(n + \frac{\Phi}{\tilde{\Phi}_0} \right)^2 + \frac{\hbar^2 k_z^2}{2m} \tag{167}$$

where Φ is the flux of the magnetic field through the cylinder, and $\tilde{\Phi}_0 = h/e$ is the so-called (normal) flux quantum.

32.2

Find the ground state quantum numbers n_0 and $k_{z,0}$. Show that the ground-state energy is a periodic function of Φ, with period $\tilde{\Phi}_0$. (*Suggestion* : look at the mathematical appendix !).

32.3

The current density associated with a wavefunction ψ reads

$$\boldsymbol{j} = -\frac{\hbar e}{2mi} (\psi^* \boldsymbol{\nabla} \psi - \psi \boldsymbol{\nabla} \psi^*) - \frac{e^2}{m} |\psi|^2 \boldsymbol{A} \ . \tag{168}$$

Calculate the current density associated with the ground state ψ_0.
Show that the ground state carries a persistent electrical current, and that this current is a periodic function of the applied flux Φ with period $\tilde{\Phi}_0$. Considering that the cylinder is equivalent to a solenoid, for which values of $\Phi/\tilde{\Phi}_0$ is the magnetic field generated by the solenoid parallel/antiparallel to the applied field $\boldsymbol{B}$?

32.4

Persistent currents in normal metals can only be observed in very special conditions. Cite at least two reasons for the decay of such currents in a normal metal. If l is the mean free path of an electron in a metal, how large does l need to be for the persistent current to be observable ?

On the other hand, as you know, persistent currents are quite stable in superconductors. In the following we will assume that the Cooper pairs appearing in a superconductor can be described by a *macroscopic wavefunction* $\Psi(\boldsymbol{r})$ (analogous to that of condensed bosons) which gives the amplitude of finding the whole condensate of Cooper pairs at point $\boldsymbol{r}$.
Moreover we will now consider a finite thickness for the cylinder, and we will assume that the superconductor develops persistent currents on the inner and outer surface of the cylinder, which screen completely the magnetic field in the bulk of the cylinder (Meissner effect). Hence the bulk of the cylinder has no magnetic field (and, consequently, zero current) – see Fig. **??**.

32.5

We will assume that the macroscopic wavefunction satisfies a similar equation to Schrödinger's equation for single particles in a magnetic field (the so-called Ginzburg-Landau equation), but this time the particle charge is $2e$ (because we have Cooper pairs). In the boundary regions, in which the magnetic field penetrates into the superconductor, we will use the results we found for the ground state of a single electron confined to a cylinder and immersed in a magnetic field. There the macroscopic wavefunction will take the form

$$\Psi(r, z, \theta) = \Psi_r(r) \ \Psi_z(z) \ \frac{1}{\sqrt{2\pi}} \exp(in\theta) \tag{169}$$

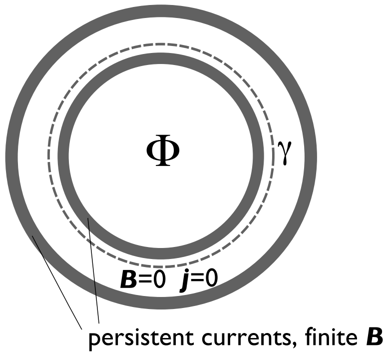


FIGURE 8 – Cross section of the superconducting cylinder.

Justify that, in the ground state

$$n = n_0(\Phi) = -\mathrm{int}\left(\frac{\Phi}{\Phi_0} + \mathrm{sign}(\Phi)\frac{1}{2}\right) \tag{170}$$

where $\Phi_0 = h/(2e)$ is the so-called superconducting flux quantum.

32.6

Going to the bulk region with zero magnetic field and current, by continuity with the boundary region we have to assume that the macroscopic wavefunction reads :

$$\Psi(r, z, \theta) = \mathcal{A}\ \frac{1}{\sqrt{2\pi}}\exp(in\theta) \tag{171}$$

where $\mathcal{A}$ is a constant. The current carried by the macroscopic wavefunction reads

$$\boldsymbol{j} = -\frac{\hbar(2e)}{2mi}\left(\Psi^*\boldsymbol{\nabla}\Psi - \Psi\boldsymbol{\nabla}\Psi^*\right) - \frac{(2e)^2}{m}|\Psi|^2\boldsymbol{A}\ . \tag{172}$$

Imposing that $\boldsymbol{j} = 0$ all along a loop γ entirely contained in the bulk region (see Fig. 3), demonstrate that the magnetic flux threading the loop obeys the *quantization condition* :

$$\Phi_\gamma = -n_0(\Phi)\Phi_0\ . \tag{173}$$

32.7

Plot the magnetic flux Φ_γ as a function of Φ/Φ_0, and compare it with the experimental results (first obtained by Deaver/Fairbank and Doll/Näbauer in 1961) for the flux trapped in the hollow of a superconducting cylinder – Fig. **??**. What is the analogous phenomenon occurring in He^4 ? Which aspect do the two systems share, which is responsible for both phenomena ?

33 Superconducting quantum interference device (SQUID)

We are used by now to the idea that the Cooper pairs in a superconductor can be described via a macroscopic wavefunction, $\Psi(\boldsymbol{r})$, such that the (super-)current flowing in a superconductor can be obtained from it as in Eq. (**??**).

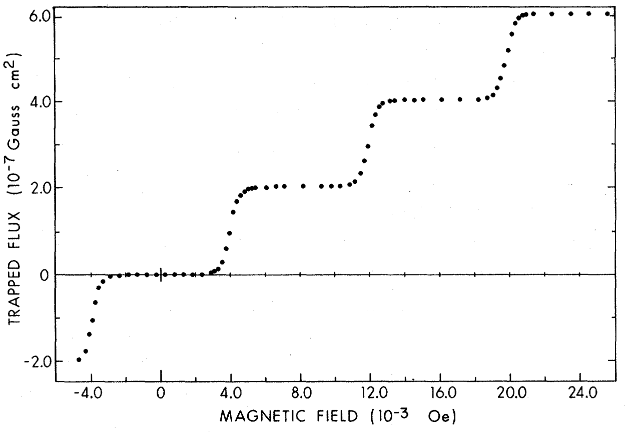


FIG. 3. Trapped flux as a function of the magnetic field in which the cylinder was cooled below its transition temperature. These data were taken with a tin cylinder, 56-μ i.d. and 24 mm long, with walls about 5000 Å thick.

FIGURE 9 – Flux quantization experiment (from W. L. Goodman *et al.*, Phys. Rev. B **4**, 1530 (1971)).

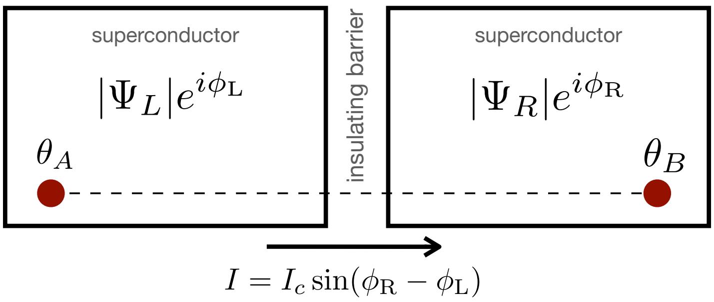


FIGURE 10 – A superconducting Josephson junction.

33.1

Using the amplitude/phase decomposition, $\Psi(\boldsymbol{r}) = |\Psi(\boldsymbol{r})|e^{i\phi(\boldsymbol{r})}$, express $\boldsymbol{j}$ as a function of $\phi(\boldsymbol{r})$. Show that if we introduce the so-called *gauge-invariant phase*

$$\theta(\boldsymbol{r}) = \phi(\boldsymbol{r}) + \frac{2e}{\hbar}\int_{\boldsymbol{r}_0}^{\boldsymbol{r}} \boldsymbol{A}\cdot d\boldsymbol{l} \tag{174}$$

then, assuming $\Psi(\boldsymbol{r}) = |\Psi(\boldsymbol{r})|e^{i\theta(\boldsymbol{r})}$, we obtain the same current if we eliminate the term proportional to $\boldsymbol{A}$ in Eq. (**??**). The line integral of the vector potential is calculated along an arbitrary line starting from the (arbitrary) point $\boldsymbol{r}_0$ – do not worry, it will become better defined later !

33.2

Let us consider now a *superconducting Josephson junction* (Fig. **??**), formed by two superconducting leads separated by a thin barrier (typically a layer of insulator). It is the exact superconducting analog of the Josephson junction we explored in the case of bosons in TD no. 5. There we saw that a tunneling current $I = I_c \sin\Delta\phi$ – going, say, from left (L) to right (R) – crosses the junction when a phase difference $\Delta\phi = \phi_{\rm R} - \phi_{\rm L}$

is present between the two macroscopic wavefunctions $\Psi_{\mathrm{L(R)}} = |\Psi_{\mathrm{L(R)}}|e^{i\phi_{\mathrm{L(R)}}}$ describing the superconductors on both sides of the junction.
When a vector potential $\boldsymbol{A}$ is present in the system, give the expression of the gauge-invariant phase difference $\theta_B - \theta_A$ between two points A and B on opposite sides of the junction.

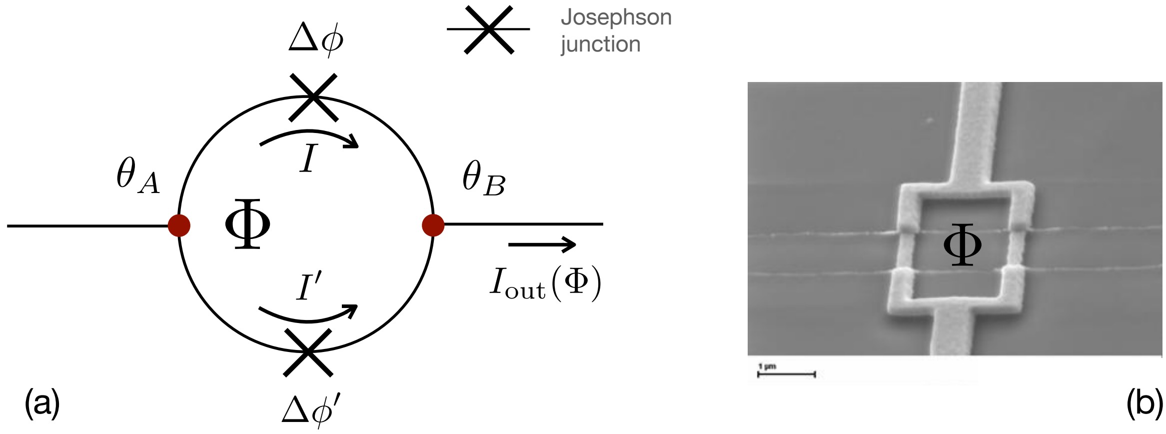


FIGURE 11 – (a) Circuit scheme of a SQUID (all the circuit elements are superconducting) ; (b) an actual SQUID (the Josephson junctions are defined by the two discontinuities in the square loop).

33.3

We now consider the circuit geometry in Fig. **??**(a), defining a so-called superconducting quantum interference device (SQUID) : two Josephson junctions are present in a superconducting loop, which is threaded with a magnetic-field flux Φ.
Using the result of the previous question for the expression of $\theta_B - \theta_A$ – this time calculated for the two points indicated in Fig. **??**(a)) – establish the relationship between the two phase differences $\Delta\phi$ and $\Delta\phi'$ across the two junctions.
Note : the line integral defining the gauge-invariant phase difference has to be taken along a circuit which runs *inside* the superconductor.

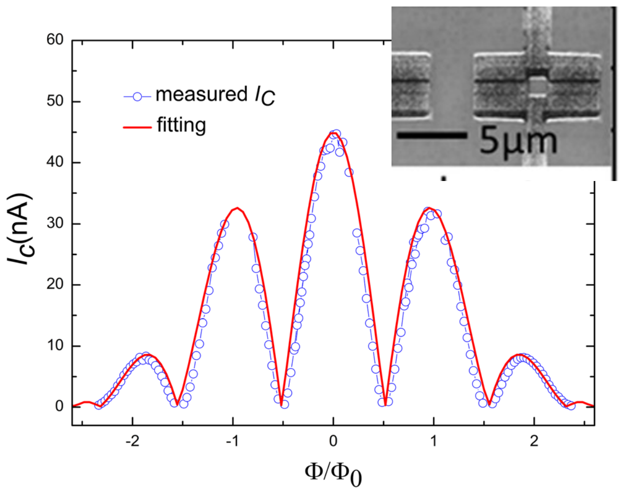


FIGURE 12 – Critical current of a micro-SQUID (from S.-S. Yeh et al., Appl. Phys. Lett. 101, 232602 (2012)).

33.4

By using Kirchhoff's law for the current, conclude that the outgoing (super-)current in the circuit takes the form

$$I_{\text{out}}(\Phi) = 2I_c \cos\left(\frac{\pi\Phi}{\Phi_0}\right) \sin(\theta_B - \theta_A) \ . \tag{175}$$

33.5

Fig. **??** shows the measured critical current through a SQUID : can you understand this result (at least partially) from the previous formula ?
This result shows that a SQUID is sensitive to magnetic fluxes of the order of Φ_0. If you have a macroscopic superconducting loop of 1mm^2, what sensitivity can you achieve on the measurement of a magnetic field ?

Note : in fact, SQUIDs can achieve a sensitivity of 1fT (10^{-15} T), which is the order of magnitude of the magnetic fields associated *e.g.* with the activity of the human brain. SQUID magnetometers are among the most sensitive ones, used broadly in many fields of research – among them, the study of brain activity.