M1- Sciences de la Matière, A. A. 2021-2022
Superconductivity, superfluidity and magnetism
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Midterm exam – March 6th, 2022 (2h)

1 Short questions

These questions only require a short answer!

Q1. Be $\hat{a}_1, \hat{a}_1^\dagger$ and $\hat{a}_2, \hat{a}_2^\dagger$ the destruction and creation operators in two single-particle states 1 and 2. Is $\hat{a}_1^\dagger \hat{a}_2 \hat{a}_2^\dagger \hat{a}_1$ a Hermitian operator? Rewrite it in terms of the number operators $\hat{n}_{1(2)} = \hat{a}_{1(2)}^\dagger \hat{a}_{1(2)}$ in the case in which $\hat{a}, \hat{a}^\dagger$ are bosonic operators, and in the case in which they are fermionic operators.

Solution: Yes, $\hat{a}_1^\dagger \hat{a}_2 \hat{a}_2^\dagger \hat{a}_1$ is Hermitian as it is of the form $\hat{A}\hat{A}^\dagger$ with $\hat{A} = \hat{a}_1^\dagger \hat{a}_2$.
Using (anti)commutation relations for bosons (fermions) one finds that $\hat{a}_1^\dagger \hat{a}_2 \hat{a}_2^\dagger \hat{a}_1 = \hat{n}_1(\pm \hat{n}_2 + 1)$ with + for bosons and - for fermions.

Q2. Consider two $S = 1/2$ particles in the following state (in first quantization):

$$\phi(x_1)\phi(x_2)\frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{\sqrt{2}}$$

where $\phi(x)$ is a single-particle wavefunction. Is it a legitimate state for two identical fermions? Write the state in second quantization using the field operators $\hat{c}_{\phi,\uparrow}^\dagger$ and $\hat{c}_{\phi,\downarrow}^\dagger$ creating a fermion in the state ϕ with spin $\uparrow$ and $\downarrow$ respectively.

Solution:

$$|\Psi\rangle = \hat{c}_{\phi,\uparrow}^\dagger \hat{c}_{\phi,\downarrow}^\dagger |0\rangle$$

Q3. Rewrite the state above by using the field operators $\hat{\psi}_\uparrow^\dagger(x)$, $\hat{\psi}_\downarrow^\dagger(x)$ creating particles with spin $\uparrow$ and $\downarrow$ at position x.

Solution:

$$|\Psi\rangle = \int dx_1 dx_2 \ \phi(x_1)\phi(x_2) \ \hat{\psi}_\uparrow^\dagger(x_1)\hat{\psi}_\downarrow^\dagger(x_2) \ |0\rangle$$

Q4. What are the assumptions underlying Bogolyubov theory for the interacting Bose gas?

Solution: One must assume that the gas is nearly 100% condensed, so that the fraction of the particles outside of the condensate can be treated as a perturbation to the fraction of the condensed particles. In the treatment that we gave in the lectures we also assumed that the atoms in the condensate are described via a macroscopic wavefunction $\Psi_0(\boldsymbol{r})$ such that the field operator writes as $\hat{\psi}(\boldsymbol{r}) = \Psi_0(\boldsymbol{r}) + \delta\hat{\psi}(\boldsymbol{r})$, with $\delta\hat{\psi}$ treated as a “perturbation” with respect to $\Psi_0(\boldsymbol{r})$.

Q5. In a rotating Bose-Einstein condensate with total vorticity of 4, order the following states depending on their energy (neglecting vortex-vortex interactions): a) two vortices with vorticity 2 each; b) three vortices with vorticity 1, 1, and 2; c) two vortices with vorticity 3 and 1. Is there a vortex state with even lower energy?

Solution: The energy of each vortex goes as the *square* of its vorticity, so that the energies are ordered as $E_b < E_a < E_c$. A state with even lower energy has 4 vortices with vorticity 1 each.

Q6. Consider the one-body density matrix $g^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = \langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}')\rangle$ for a system of identical bosons. What is the value of this function for $|\boldsymbol{r} - \boldsymbol{r}'| \to 0$? And what is its behavior for $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$ in the absence of Bose condensation?

Solution: $g^{(1)}(\boldsymbol{r}, \boldsymbol{r}) = n$ (average density). $g^{(1)}(\boldsymbol{r}, \boldsymbol{r}')$ decays to zero when $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$ in the absence of condensation.

2 Hydrogen atom as a composite boson

Let us consider two types of fermions, electrons and protons, with associated quantum fields $\hat{\psi}_e(\boldsymbol{r}), \hat{\psi}_e^\dagger(\boldsymbol{r})$ and $\hat{\psi}_p(\boldsymbol{r}), \hat{\psi}_p^\dagger(\boldsymbol{r})$, respectively. In the following we shall neglect the fact that electrons and protons carry a spin, which is not relevant for the present discussion.

2.1

For identical fermions we have the anticommutation relations

$$\{\hat{\psi}_e(\boldsymbol{r}), \hat{\psi}_e^\dagger(\boldsymbol{r}')\} = \delta(\boldsymbol{r} - \boldsymbol{r}') \qquad \{\hat{\psi}_e(\boldsymbol{r}), \hat{\psi}_e(\boldsymbol{r}')\} = 0$$

and the same holds for the protons ($e \to p$). Justify why instead we can write

$$[\hat{\psi}_e(\boldsymbol{r}), \hat{\psi}_p^\dagger(\boldsymbol{r}')] = [\hat{\psi}_e(\boldsymbol{r}), \hat{\psi}_p(\boldsymbol{r}')] = 0 \ .$$

Solution: Because electrons and protons are mutually distinguishable! I can have a proton and an electron in the same state, even though they are fermions.

2.2

Consider now the hydrogen atom, which is a bound state of a proton and an electron. Be $\phi_0(\boldsymbol{r})$ the ground-state wavefunction of the hydrogen atom for the relative coordinate $\boldsymbol{r}$ (namely the distance between the proton and the electron). Justify why the "hydrogen operator"

$$\hat{h}_0^\dagger(\boldsymbol{R}) = \int d^3r \ \phi_0(\boldsymbol{r}) \ \hat{\psi}_e^\dagger(\boldsymbol{r} + \boldsymbol{R}) \ \hat{\psi}_p^\dagger(\boldsymbol{R}) \tag{1}$$

creates a hydrogen atom in its electronic ground state with the nucleus at position $\boldsymbol{R}$.

Solution: $\hat{\psi}_p^\dagger(\boldsymbol{R})$ creates the nucleus at the desired position; $\int d^3r \ \phi_0(\boldsymbol{r}) \ \hat{\psi}_e^\dagger(\boldsymbol{r} + \boldsymbol{R}) = \hat{c}^\dagger_{\phi_0, \boldsymbol{R}}$ creates an electron in the state ϕ_0 centered around $\boldsymbol{R}$.

2.3

We want to study the commutation relations of the $\hat{h}_0(\boldsymbol{R}), \hat{h}_0^\dagger(\boldsymbol{R})$ operators. Calculate the commutation bracket

$$[\hat{\psi}_p(\boldsymbol{R})\ \hat{\psi}_e(\boldsymbol{R}+\boldsymbol{r}), \psi_e^\dagger(\boldsymbol{R}'+\boldsymbol{r}')\ \hat{\psi}_p^\dagger(\boldsymbol{R}')]\ . \tag{2}$$

(*Suggestion:* try to rewrite $\psi_e^\dagger(\boldsymbol{R}'+\boldsymbol{r}')\ \hat{\psi}_p^\dagger(\boldsymbol{R}')\hat{\psi}_p(\boldsymbol{R})\ \hat{\psi}_e(\boldsymbol{R}+\boldsymbol{r})$ in terms of $\hat{\psi}_p(\boldsymbol{R})\ \hat{\psi}_e(\boldsymbol{R}+\boldsymbol{r})\psi_e^\dagger(\boldsymbol{R}'+\boldsymbol{r}')\ \hat{\psi}_p^\dagger(\boldsymbol{R}')$ by using the known anticommutation relations of fermions).

Solution: The result is

$$-\delta(\boldsymbol{R}-\boldsymbol{R}')\ \hat{\psi}_e^\dagger(\boldsymbol{r}'+\boldsymbol{R}')\ \hat{\psi}_e(\boldsymbol{r}+\boldsymbol{R}) + \delta(\boldsymbol{r}'+\boldsymbol{R}'-\boldsymbol{r}-\boldsymbol{R})\ \hat{\psi}_p(\boldsymbol{R})\ \hat{\psi}_p^\dagger(\boldsymbol{R}')$$

2.4

Conclude that

$$[\hat{h}_0(\boldsymbol{R}), \hat{h}_0^\dagger(\boldsymbol{R}')] = -\hat{c}_{\phi_0,\boldsymbol{R}}^\dagger \hat{c}_{\phi_0,\boldsymbol{R}}\ \delta(\boldsymbol{R}-\boldsymbol{R}') + \int d^3r\ \phi_0(\boldsymbol{r})\phi_0(\boldsymbol{r}+\boldsymbol{R}-\boldsymbol{R}')\ \hat{\psi}_p(\boldsymbol{R})\hat{\psi}_p^\dagger(\boldsymbol{R}')$$

where we have introduced the operator

$$\hat{c}_{\phi_0,\boldsymbol{R}}^\dagger = \int d^3r\ \phi_0(\boldsymbol{r})\ \hat{\psi}_e^\dagger(\boldsymbol{r}+\boldsymbol{R})$$

and we have assumed that $\phi_0 \in \mathbb{R}$ (as it is the case).

Solution: It just follows by integrating the result of the previous section over $\boldsymbol{r}$ and $\boldsymbol{r}'$.

2.5

The ground-state hydrogen wavefunction has a linear spatial extent of about a Bohr radius, $a_0 \approx 0.5 \times 10^{-10}$ m. Under which physical conditions can one have that $[\hat{h}_0(\boldsymbol{R}), \hat{h}_0^\dagger(\boldsymbol{R}')] \approx 0$? What can you conclude about the possibility of treating hydrogen atoms as bosons?

Solution: The commutation relation vanishes when $\boldsymbol{R} \neq \boldsymbol{R}'$ (for the first term) and when $|\boldsymbol{R}-\boldsymbol{R}'| \gg a_0$ (to let the second term vanish), which also implies the vanishing of the first term *a fortiori*. Hence two hydrogen atoms behave as composite bosons (namely, their operators commute) when they stay at a distance much bigger than their spatial extent.

3 Bosonic bunching and the effect of interactions on a BEC

In this section we would like to evaluate the effect of interactions on a Bose gas in the case in which it is condensed or not.

To do so, we shall evaluate the so called $g^{(2)}(0)$ function, which reads

$$g^{(2)}(0) = \frac{\langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\rangle}{\langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\rangle^2} \tag{3}$$

where $\hat{\psi}(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r})$ are bosonic field operators.

3.1

Introducing the destruction operator in momentum space

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

write $\langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\rangle$ in terms of the 4-momentum expectation value $\langle \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{q}}\hat{a}_{\boldsymbol{k}'}\hat{a}_{\boldsymbol{q}'}\rangle$. Conclude that, if the system is translationally invariant (namely momentum must be conserved), then $\langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\rangle$ is independent of $\boldsymbol{r}$.

Solution:

$$\langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\rangle = \frac{1}{V^2}\sum_{\boldsymbol{k}\boldsymbol{q}}\sum_{\boldsymbol{k}'\boldsymbol{q}'} e^{-i(\boldsymbol{k}+\boldsymbol{q}-\boldsymbol{k}'-\boldsymbol{q}')\cdot\boldsymbol{r}} \langle \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{q}}\hat{a}_{\boldsymbol{k}'}\hat{a}_{\boldsymbol{q}'}\rangle \ .$$

With momentum conservation, one must have $\boldsymbol{k}+\boldsymbol{q} = \boldsymbol{k}'+\boldsymbol{q}'$, so that the spatial dependence drops out.

3.2

In the case of an ideal Bose gas, we have that all states which enter in the averages $\langle ... \rangle$ have a well-defined number of particles $\{n_{\boldsymbol{p}}\}$ in each single-particle state with wave-vector $\boldsymbol{p}$. This means that one should consider only quartets of wavevectors $\boldsymbol{k},\boldsymbol{q},\boldsymbol{k}',\boldsymbol{q}'$ such that $\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{q}}\hat{a}_{\boldsymbol{k}'}\hat{a}_{\boldsymbol{q}'}|\{n_{\boldsymbol{p}}\}\rangle = c|\{n_{\boldsymbol{p}}\}\rangle$, where c is a proportionality constant.

Conclude that

$$\langle \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{q}}\hat{a}_{\boldsymbol{k}'}\hat{a}_{\boldsymbol{q}'}\rangle = n_{\boldsymbol{k}}(n_{\boldsymbol{q}} - \delta_{\boldsymbol{k},\boldsymbol{q}})\left[\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\boldsymbol{q},\boldsymbol{q}'} + \delta_{\boldsymbol{k},\boldsymbol{q}'}\delta_{\boldsymbol{k}',\boldsymbol{q}}(1-\delta_{\boldsymbol{k},\boldsymbol{q}})\right]$$

where $n_{\boldsymbol{k}} = \langle \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\rangle$.

Solution: Only the combinations $\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{q}}\hat{a}_{\boldsymbol{q}}\hat{a}_{\boldsymbol{k}}$ and $\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{q}}\hat{a}_{\boldsymbol{k}}\hat{a}_{\boldsymbol{q}}$ count; but one has to avoid counting twice the case with all equal wavevectors, which appears in principle in both cases (hence the factor $(1-\delta_{\boldsymbol{k},\boldsymbol{q}})$).

3.3

In the case of a perfect BEC, $n_{\boldsymbol{k}} = N\delta_{\boldsymbol{k},0}$, show that

$$g^{(2)}(0) = 1 + \mathcal{O}\left(\frac{1}{V}\right) \ .$$

Solution: One has that for the ideal Bose gas

$$\langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\rangle = \frac{1}{V^2}\sum_{\boldsymbol{k}\boldsymbol{q}}(n_{\boldsymbol{k}}n_{\boldsymbol{q}} - n_{\boldsymbol{k}}\delta_{\boldsymbol{k},\boldsymbol{q}})(2-\delta_{\boldsymbol{k},\boldsymbol{q}}) = 2n^2 - \frac{1}{V^2}\sum_{\boldsymbol{k}} n^2_{\boldsymbol{k}} - \frac{n}{V} \ .$$

In the case of a condensate $\frac{1}{V^2}\sum_{\boldsymbol{k}} n^2_{\boldsymbol{k}} = n^2$, so that $\langle \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\rangle = n^2 + O(1/V)$.

3.4

We consider then the opposite limit of a gas with a rather flat momentum distribution (non-condensed gas), namely $n_{\boldsymbol{k}} \sim O(1)$ for N wavevectors. Show then that

$$g^{(2)}(0) = 2 + \mathcal{O}\left(\frac{1}{V}\right) \ .$$

This effect for the non-condensed Bose gas is called *bosonic bunching* – and it expresses the fact that if one finds a boson in a given position in space it is twice more likely to find a second one than in a system of spatially uncorrelated particles.

Solution: In this case $\frac{1}{V^2}\sum_{\boldsymbol{k}} n_{\boldsymbol{k}}^2 \approx n/V$, and the result follows.

3.5

The above result has strong consequences in terms of the stability of a condensate to interactions. Considering the potential energy due to a contact potential

$$\hat{\mathcal{H}}_{\rm int} = \frac{g}{2}\int d^3r \ \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})$$

calculate the expectation value of this energy on the perfect BEC and for the non-condensed gas. Which state has the lowest potential energy?

Solution:

$$\langle\hat{\mathcal{H}}_{\rm int}\rangle = \begin{cases} \frac{gn}{2}N + O(1/V) & \text{BEC} \\ gnN + O(1/V) & \text{non} - \text{BEC} \end{cases} \ .$$

Clearly the BEC case has the lowest potential energy.