M1- Sciences de la Matière, A. A. 2022-2023
Superconductivity, superfluidity and magnetism
Tommaso Roscilde, Fabio Mezzacapo, Youssef Trifa

Midterm exam – March 6th, 2023 (2h)

1 Short questions

These questions only require a short answer/ a short calculation!

Q1. Normal ordering of operator products in second quantization (denoted as : ... :) amounts to rewriting such products by putting all the creation operators to the left of the destruction ones. For instance, for two bosonic modes 1 and 2, $: b_1 b_2^\dagger := b_2^\dagger b_1$. Calculate the difference between $b_1^\dagger b_2 b_1 b_2^\dagger$ and $: b_1^\dagger b_2 b_1 b_2^\dagger :$; and the expectation value $\langle 0| : b_1^\dagger b_2 b_1 b_2^\dagger : |0\rangle$ on the vacuum state $|0\rangle$.

> **Solution:** $b_1^\dagger b_2 b_1 b_2^\dagger - : b_1^\dagger b_2 b_1 b_2^\dagger := b_1^\dagger b_1$
> $\langle 0| : b_1^\dagger b_2 b_1 b_2^\dagger : |0\rangle = 0$ (as for any normal-ordered product)

Q2. Consider the two states (in first quantization) for two particles:

$$|\pm\rangle = \frac{|\psi\rangle|\phi\rangle \pm |\phi\rangle|\psi\rangle}{\sqrt{2}} \ . \qquad (1)$$

Rewrite these two states using bosonic operators $b_\psi^\dagger, b_\phi^\dagger$ and/or fermionic operators $c_\psi^\dagger, c_\phi^\dagger$ acting on the vacuum.

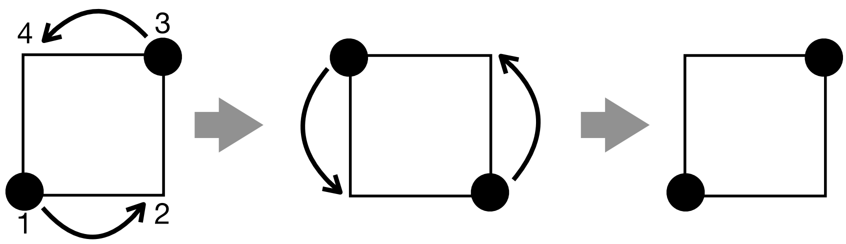
> **Solution:**
> $$|+\rangle = b_\psi^\dagger b_\phi^\dagger |0\rangle \qquad |-\rangle = c_\psi^\dagger c_\phi^\dagger |0\rangle$$

Q3. Using creation and destruction operators, write an operator which destroys a particle with wavevector $\boldsymbol{k}$ and creates two identical particles to the first one, with wavevectors $\boldsymbol{k}+\boldsymbol{q}$ and $\boldsymbol{k}-\boldsymbol{q}$. Which particles in physics could experience such a transformation?

> **Solution:** $b_{\boldsymbol{k}+\boldsymbol{q}}^\dagger b_{\boldsymbol{k}-\boldsymbol{q}}^\dagger b_{\boldsymbol{k}}$. This process cannot happen using massive particles, because mass would not be conserved. On the other hand it may happen with quasiparticles, such as phonons or magnons; or massless particles such as photons.

Q4. Consider a system of 2 fermions on a 4-site square, as depicted in the figure below. Using second quantization, we want to describe the mathematical operations that exchange the two particles.

Be c_1, c_2, c_3, and c_4 the operators that destroy a particle in the sites 1, 2, 3 and 4, while $c_1^\dagger$, $c_2^\dagger$, $c_3^\dagger$, and $c_4^\dagger$ are the ones creating a particle. We imagine that particles can be made to hop only between nearest-neighboring sites, by using the hopping operators $c_2^\dagger c_1$, $c_3^\dagger c_2$, $c_4^\dagger c_3$ and $c_1^\dagger c_4$. Using hopping operators applied to the initial state $|n_1, n_2, n_3, n_4\rangle = |1, 0, 1, 0\rangle$ as in the sequence described in the figure, show that one comes back to the same state, but with a minus sign in front.



Solution: The sequence is described by $c_1^\dagger c_4 c_3^\dagger c_2 c_2^\dagger c_1 c_4^\dagger c_3 |1,0,1,0\rangle = -c_1^\dagger c_1 c_4 c_4^\dagger c_3^\dagger c_3 c_2 c_2^\dagger |1,0,1,0\rangle = -|1,0,1,0\rangle$

Q5. For an ideal Bose gas, Bose-Einstein condensation is possible at finite temperature in $d = 2$ dimensions. True or false? Can you motivate your answer with a small calculation?

Solution: It is false, because the number of atoms in the excited states can diverge for zero chemical potential since it goes as $\tilde{N}_{\max} \sim \int dk\ k^{d-1}/[\exp(\hbar^2 k^2/(2m)) - 1] \sim \int dk\ k^{d-3}$, diverging for $d = 1$ and 2.

2 Squeezed states of a harmonic oscillator

We consider a single harmonic oscillator (or equivalently a single bosonic mode), described in terms of the destruction/creation operators a, $a^\dagger$; and its so-called *squeezed* states. To generate squeezed states, one uses the squeezing operator

$$S(r) = e^{\frac{r}{2}\left[(a^\dagger)^2 - a^2\right]} \tag{2}$$

where r is a real number.

2.1

Show that $S(r)$ is unitary.

Solution: $S^\dagger(r) = S(-r)$ so that $S^\dagger(r)S(r) = 1$.

2.2

We consider the unitarily transformed operator a:

$$b(r) = S^\dagger(r)\ a\ S(r)\ . \tag{3}$$

Write the expression of $b^\dagger(r)$, and of the derivative $db(r)/dr$ in terms of $b(r), b^\dagger(r)$.

Solution:

$$b^\dagger(r) = S^\dagger(r)\ a^\dagger\ S(r)$$
$$\frac{db}{dr} = b^\dagger(r)$$

2.3

Show that the equation for $db(r)/dr$, with the condition $b(0) = a$, admits the solution

$$b(r) = \cosh(r)\ a + \sinh(r)\ a^\dagger \tag{4}$$

Prove that $b, b^\dagger$ are still bosonic operators.

Solution:

$$\frac{db}{dr} = b^\dagger(r) = \sinh(r)\ a + \cosh(r)\ a^\dagger = b^\dagger(r)$$

and $b(0) = a$ indeed. b and $b^\dagger$ are bosonic operators because $[b, b^\dagger] = \cosh^2(r) - \sinh^2(r) = 1$.

2.4

Consider the so-called *squeezed vacuum state*, given by $|r\rangle = S(r)|0\rangle$.
Calculate the average particle number $n(r) = \langle r|a^\dagger a|r\rangle$, and its behavior for $r \to \pm\infty$. Is this still the vacuum?

Solution:

$$\langle r|a^\dagger a|r\rangle = \langle 0|b^\dagger(r)b(r)|0\rangle = \langle 0|\left[c^2 a^\dagger a + s^2 a a^\dagger + cs(a^\dagger a^\dagger + a^2)\right]|0\rangle = \sinh^2(r) \sim_{r\to\pm\infty} \frac{e^{2|r|}}{4}\ .$$

This is clearly not the vacuum, because the number is growing exponentially with $|r|$.

2.5

We introduce the (dimensionless) position and momentum operators $X = (a + a^\dagger)/\sqrt{2}$ and $P = (a - a^\dagger)/(i\sqrt{2})$. Calculate $\langle r|X|r\rangle$, $\langle r|P|r\rangle$, $\langle r|X^2|r\rangle$ and $\langle r|P^2|r\rangle$.

Solution:

$$\langle X\rangle_r = \langle P\rangle_r = 0\ ;$$

$$\langle X^2\rangle_r = \frac{1}{2}\langle 0|(b + b^\dagger)^2|0\rangle = \frac{1}{2}(c+s)^2 = \frac{e^{2r}}{2}\ ;$$
$$\langle P^2\rangle_r = -\frac{1}{2}\langle 0|(b - b^\dagger)^2|0\rangle = \frac{1}{2}(c-s)^2 = \frac{e^{-2r}}{2}$$

2.6

Calculate the product $(\Delta X)_r(\Delta P)_r$, where $(\Delta X)_r = \sqrt{\langle r|X^2|r\rangle - \langle r|X|r\rangle^2}$ and similarly for $(\Delta P)_r$. Does this product change with respect to the vacuum $|r = 0\rangle$? When $r \to \infty$, can you recognize an operator of which the squeezed vacuum becomes an eigenstate?

Solution: $(\Delta X)_r(\Delta P)_r = 1/2$ as in the vacuum. For $r \to \infty$, $(\Delta P)_r = e^{-r}/\sqrt{2} \to 0$, namely the squeezed state tends to a momentum eigenstate.

3 XXZ model of ferromagnetism: spin-wave theory vs. mean-field theory

In this exercise, we consider the XXZ model of ferrromagnetism, whose Hamiltonian reads

$$\begin{aligned}\mathcal{H} &= -\frac{J}{2}\sum_i\sum_{\boldsymbol{d}}\left[S_i^x S_{i+\boldsymbol{d}}^x + S_i^y S_{i+\boldsymbol{d}}^y + \Delta S_i^z S_{i+\boldsymbol{d}}^z\right] - H\sum_i S_i^z \\ &= -\frac{J}{2}\sum_i\sum_{\boldsymbol{d}}\left[\frac{1}{2}(S_i^+ S_{i+\boldsymbol{d}}^- + S_i^- S_{i+\boldsymbol{d}}^+) + \Delta S_i^z S_{i+\boldsymbol{d}}^z\right] - H\sum_i S_i^z \end{aligned} \tag{5}$$

where Δ is an anisotropy parameter, which introduces a difference between the interaction energy for the x and y spin components, and that for the z spin components. We have also introduced a magnetic field H. Otherwise $J > 0$ is the interaction energy; the index i runs on the sites of a d-dimensional hypercubic lattice (a linear chain for $d = 1$; a square lattice for $d = 2$; and a cubic lattice for $d = 3$) comprising $N = L^d$ sites; and $\boldsymbol{d}$ is the vector connecting the site i to its $z = 2d$ nearest neighbors.

3.1

Introducing the (linearized) Holstein-Primakoff transformation

$$S^z = S - b^\dagger b \qquad S^+ \approx \sqrt{2S}\; b \qquad S^- \approx \sqrt{2S}\; b^\dagger \tag{6}$$

rewrite the above Hamiltonian in terms of the bosonic operators $b, b^\dagger$.

Solution:

$$\mathcal{H} \approx -\frac{1}{2}JzN\Delta S^2 - NHS - \frac{JS}{2}\sum_{i,\boldsymbol{d}}\left(a_i^\dagger a_{i+\boldsymbol{d}} + a_{i+\boldsymbol{d}}^\dagger a_i\right) + (H + JSz\Delta)\sum_i n_i$$

3.2 (Bonus question)

Introducing the Fourier-transformed bosons

$$b_i = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} b_{\boldsymbol{k}} \tag{7}$$

show that one can rewrite the Hamiltonian as

$$\mathcal{H} = \sum_{\boldsymbol{k}} f_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}} + \text{const.} \tag{8}$$

where $f_{\boldsymbol{k}} = -zJS\gamma_{\boldsymbol{k}} + JSz\Delta + H$, and $\gamma_{\boldsymbol{k}} = z^{-1}\sum_{\boldsymbol{d}} e^{i\boldsymbol{k}\cdot\boldsymbol{d}} = \frac{1}{d}\left(\cos(k_x) + ... + \cos(k_d)\right)$.

3.3

We start from the result of the previous question. Show that $\gamma_{\boldsymbol{k}} = 1 - k^2/z$, so that, for small k, the above Hamiltonian can be rewritten as $\mathcal{H} = \sum_{\boldsymbol{k}}(e_{\boldsymbol{k}} - \mu)b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}} + \text{const.}$ where $e_{\boldsymbol{k}} = Ak^2$ (with A a constant to be specified); and μ is a chemical potential to be calculated.

Solution: $a = JS$; $\mu = JSz(1 - \Delta) - H$.

3.4

Show that the density of Holstein-Primakoff bosons (number of bosons per lattice site) at inverse temperature $\beta = 1/(k_B T)$ can be written as

$$n_b = \frac{N_b}{N} = \frac{\Omega_d}{(2\pi)^d}\left(\frac{k_B T}{JS}\right)^{d/2}\int_0^\infty dx \frac{x^{d-1}}{e^{x^2}\zeta^{-1}-1} \tag{9}$$

where $\zeta = e^{\beta\mu}$, and Ω_d is the solid angle in d dimensions. If $\mu < 0$, in the limit $T \to 0$ ($\beta \to \infty$) show that

$$n_b \approx \frac{\Omega_d}{(2\pi)^d} I_d \left(\frac{k_B T}{JS}\right)^{d/2} e^{-\beta|\mu|} \tag{10}$$

where I_d is a convergent integral.

Solution:

$$n_b = \frac{1}{V}\sum_{\boldsymbol{k}} \frac{1}{e^{\beta(e_{\boldsymbol{k}}-\mu)}-1} = \frac{\Omega_d}{(2\pi)^d}\int_0^\infty dk\, \frac{k^{d-1}}{e^{\beta(JSk^2-\mu)}-1}$$

which gives the integral above when setting $x = \sqrt{\beta JS}k$. When $\beta \to \infty$, $e^{\beta(JSk^2-\mu)} - 1 \approx e^{\beta JSk^2}e^{\beta|\mu|}$, hence the integral

$$I_d = \int_0^\infty dx\; x^{d-1}e^{-x^2} = \frac{1}{2}\Gamma(d/2)$$

which is a convergent Gaussian integral, with $\Gamma(d/2) = \sqrt{\pi}, 1, \sqrt{\pi}/2$ for $d = 1$, 2, and 3, respectively.

3.5

We consider now the average magnetization per spin,

$$m(T) = \frac{1}{N}\sum_i \langle S_i^z \rangle \;. \tag{11}$$

Justify that $m(T) = S - n_b$ within spin-wave theory.

On the other hand, within mean-field theory for the XXZ model

$$m(T) = S\; \mathcal{B}_S[\beta(JS\Delta zm + H)] \;. \tag{12}$$

Given that $\mathcal{B}_S(x \to \infty) \approx 1 - e^{-x/S}/S$, and $m(T) \to S$ for $T \to 0$, compare the mean-field expression and the spin-wave one for $m(T)$ when $\beta \to \infty$. Do they predict the same behavior? Can you imagine a limit in which the dominant temperature dependence of $m(T)$ is the same?

Solution: $m(T) = S - n_b$ within spin-wave theory because $S_i^z = S - \langle b_i^\dagger b_i \rangle$. We have that

$$m(T) = S - \frac{\Omega_d}{(2\pi)^d} I_d \left(\frac{k_B T}{JS}\right)^{d/2} e^{-\beta[JS(\Delta-1)z+H]}$$

from spin-wave theory, while

$$m(T) = S - e^{-\beta(JSz\Delta+H)}$$

from mean-field theory. Hence the exponential temperature dependence is well captured by mean-field theory, but the dependence on the anisotropy is wrong – it should be $\Delta - 1$ instead of Δ. On the other hand the field dependence is correct; hence if $H \gg JS\Delta$, the the dependence as $\exp(-\beta H)$ of the magnetization emerges in both theories.

3.6

Consider now the case $H = 0$. In the TD no. 2, you learned that, if $\Delta = 1$, there is no ferromagnetism at $T > 0$ in $d = 1, 2$ (can you remember why?). What condition on Δ guarantees that ferromagnetism survives also in $d = 1, 2$?

Solution: We see here that, as long as $\mu < 0$, ferromagnetism can persist at finite (albeit possibly small) temperatures. If $H = 0$, $\Delta > 1$ guarantees that $\mu < 0$. If $\Delta = 1$, on the other hand, the integral of Eq. (9) diverges for $d = 1, 2$.

3.7

Calculate the susceptibility $\chi = \frac{dm}{dH}$ within spin-wave theory, and take the limit $H = 0$. Do you understand why, for $\Delta > 1$ the susceptibility becomes exponentially small when $T \to 0$?

Solution:

$$\chi = \beta \frac{\Omega_d}{(2\pi)^d} I_d \left(\frac{k_B T}{JS} \right)^{d/2} e^{-\beta[JS(\Delta-1)z+H]} .$$

The susceptibility vanishes exponentially for $T \to 0$ because the magnetization is reaching its saturation value exponentially as well, and applying a magnetic field cannot make it increase any further.

3.8

And what about $\Delta < 1$? Does the result for $m(T)$ in spin-wave theory still make sense? If not, can you understand what kind of ferromagnetic order you should expect from the ground state of the Hamiltonian in Eq. (5)? And what does mean-field theory say in this case? What is the condition for the mean-field prediction to become unstable?

Solution: For $\Delta < 1$, $m(T)$ goes to $-\infty$ exponentially when $T \to 0$, which is absurd. This is indicative of the fact that the theory assumes order along the z axis, but this order is not at all verified. Indeed for $\Delta < 1$ the ground state of the Hamiltonian Eq. (5) develops rather ferromagnetic order in the xy plane, while ferromagnetism along z becomes unstable. Mean-field theory instead is not sensitive to the fact that $\Delta < 1$, and it still provides a self-consistent solution even in this case. For mean-field theory to signal its breakdown we need the stronger condition $\Delta < 0$, such that the mean-field magnetization also goes to $-\infty$ when $T \to 0$. In this case in fact the z spin components interact antiferromagnetically, so that ferromagnetism for the z spin components becomes unstable even at the mean-field level.