E8.1 *Foundations of statistical physics, Bose–Einstein condensation*

Particle with Spin $S$ confined to a box $B = \{ \vec{r} \in \mathbb{R}^3 \, | \, 0 \leq x_k \leq L \}$ with length $L$ and volume $V = L^3$ have wave functions $\{ \chi^{(\sigma)} \}$ a spinor:

$$\psi^{(\sigma)}(\vec{r}) = \frac{1}{\sqrt{V}} e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \chi^{(\sigma)}(\vec{r}), \quad \vec{p} = \frac{2\pi \hbar}{L}, \quad \vec{r} \in \mathbb{Z}^3, \quad \sigma = -S, \ldots, S.$$

The $\psi^{(\sigma)}$ are periodic: $\psi^{(\sigma)}(L\vec{n}) = \psi^{(\sigma)}(0)$ and form an orthonormal basis for the functions in $B: \int_{B} d^3 r \psi^{(\sigma)^*}(\vec{r}) \psi^{(\sigma')}(\vec{r'}) = \delta_{\vec{r} \vec{r'}} \delta_{\sigma \sigma'}$. The $N-$particle states in 2nd quantisation are $\frac{1}{\sqrt{N!}} (\prod_{i=1}^{N} a^{\dagger}_{\vec{n}_i, \sigma_i}) |0\rangle$. Number and energy operator read $N = \sum_{\vec{n}, \sigma} a^{\dagger}_{\vec{n}, \sigma} a_{\vec{n}, \sigma}$ and $H = \sum_{\vec{n}, \sigma} \varepsilon(\vec{n}) a^{\dagger}_{\vec{n}, \sigma} a_{\vec{n}, \sigma}$. The statistical operator $\varrho$ (density operator) is given by

$$\varrho = \frac{1}{Z} e^{-\beta(H-\mu N)}, \quad Z = \text{Spur } e^{-\beta(H-\mu N)} \quad (\Rightarrow \text{Spur } \varrho = 1).$$

$Z$ is called partition function, $\mu$ chemical potential and with the temperature $T$ and Boltzmann’s constant $k$ one has $\beta = \frac{1}{kT}$. The two “Lagrang multipliers” $\mu$ and $\beta$ adjust the particle number and the energy. $\mu$ is the energy one needs (or gains) to add a particle to the system. In general, every thermodynamic quantity is given by the expectation value of an operator $\mathcal{O}$ as $\langle \mathcal{O} \rangle := \text{Tr}(\mathcal{O} \varrho)$.

In H7.2 we had: $Z = \prod_{\vec{n}} (1 + e^{-\beta(\varepsilon(\vec{n}) - \mu)})^{\pm g}$, $g = 2S + 1$ and $\langle n_{\vec{n}, \sigma} \rangle = \frac{1}{e^{\beta(\varepsilon(\vec{n}) - \mu)} - 1}$ for the average occupation of the state $\langle \vec{n}, \sigma \rangle$, where “+” is taken for fermions. We define the mean particle number $\bar{N} = \sum_{\vec{n}, \sigma} \langle n_{\vec{n}, \sigma} \rangle$ and energy $\bar{E} = \sum_{\vec{n}, \sigma} \varepsilon(\vec{n}) \langle n_{\vec{n}, \sigma} \rangle$.

1. Why is $\mu \leq 0$ for bosons? Is there a restriction on $\mu$ in the fermionic case?

2. Establish the replacement $\sum_{\vec{n}, \sigma} \rightarrow g \frac{V}{(2\pi \hbar)^2} \int d^3 p$ in the continuum limit $V \rightarrow \infty$.

Show that the limits for $V \rightarrow \infty$ of $\frac{\bar{E}}{V}$, $\frac{\bar{N}}{V}$ and $\ln \frac{Z}{V}$ do exist and compute them for $\varepsilon(\vec{p}) = \frac{1}{2m} \vec{p}^2$. Introduce the Fermi and Bose functions

$$\begin{cases} f_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty dx \frac{x^{\nu-1}}{e^x \mp 1} \\ g_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty dx \frac{x^{\nu-1}}{e^x \mp 1} \end{cases}.$$  

Which famous function of $n \in \mathbb{N}$ from number theory is $g_n(z = 1)$?

3. Show $\bar{E} = \frac{3}{2\beta} \ln Z$ and compute the classical limit, defined in such a way that $z := e^{\mu/kT} \ll 1$. $z$ is called fugacity. State this condition in the form $\lambda^3 \ll \frac{V}{\bar{N}}$ with the thermal wave length $\lambda = \hbar \sqrt{2\pi \beta / m}$ and interpret it.

4. Show that for the grand canonical potential $\Phi := -\beta^{-1} \ln Z$ one has $\Phi = -p V$. $p := -\frac{\partial \Phi}{\partial V}$ is the pressure. For that purpose show $p = \frac{2\bar{E}}{3V}$, before taking $V \rightarrow \infty$.

5. In the fermionic case at $T = 0$ the lowest energy levels are occupied once. The maximal momentum is called Fermi momentum $\vec{p}_F$, the energy $\frac{\vec{p}_F^2}{2m}$ Fermi energy $E_F$. Show $\bar{N} = \frac{g \nu V \vec{p}_F^3}{6\pi^2 \hbar^3}$ and deduce $\bar{E} = \frac{3}{2} E_F \bar{N}$. Argue that $\mu = E_F$. 

Exercises VIII

December 10th
As an important application of the general considerations we consider a nonrelativistic Bose gas with spin 0 for small temperatures $T$.

(6) Why is the fugacity bounded by $z \leq 1$? Show that $\frac{\lambda^3 N}{V} = g_{3/2}(z)$.

(7) Show that $z = 1$ is reached at a critical temperature $T_c$, defined by

$$kT_c = \frac{2\pi \hbar^2 N^{2/3}}{m(g_{3/2}(1)V)^{2/3}}.$$ 

(8) By considering the ground state separately, show that $z = 1$ is reached at a critical temperature $T_c$ defined by

$$kT_c = 2\frac{\frac{\lambda}{\sqrt{2}}}{\hbar} N^2 \frac{3}{m(g_{3/2}(1))}. $$

(9) Deduce that for $T < T_c$ the ground state is occupied macroscopically, i.e.,

$$\lim_{N \to \infty, \frac{N_0}{N} \to 0} \frac{N_0}{N} = 0 \quad T > T_c \quad \text{and} \quad \frac{N_0}{N} = 1 \quad T < T_c \quad \text{("thermodynamic limit")}. $$

Also show that the other states can never be occupied macroscopically.

(10) Why is this condensation possible only for spatial dimension $d \geq 3$?

This effect was predicted in 1924 by A. Einstein following statistical observations of S. Bose. It was observed experimentally in 1995 using alcali atoms (mostly rubidium) in a quadrupole trap with $T = 0.17\mu K$, in 1998 also with atomic hydrogen.

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**Homework VIII**

Return: Dezember 17th

H8.1 *Bardeen–Cooper–Schrieffer theory*

This theory (nobel price 1972) explains the superconductivity of 1st kind by so-called Cooper pairs, i.e. correlated electrons pairs with spin 0, for which the electric resistance vanishes. The model considers two-electron excitations $|\Phi\rangle$ of the vacuum $|0\rangle$.

The Hamiltonian of a many electrons system in a solid state reads

$$H = \sum_{\vec{k}, \sigma} \varepsilon(\vec{k}) a_{\vec{k}, \sigma}^+ a_{\vec{k}, \sigma} - \frac{1}{2} \sum_{\vec{k}, \vec{k}', \vec{w}, \sigma, \sigma'} v_{\vec{k}, \vec{k}', \vec{w}} a_{\vec{k}+\vec{w}, \sigma}^+ a_{\vec{k}', \sigma'}^+ a_{\vec{k}', \sigma} a_{\vec{k}+\vec{w}, \sigma}.$$ 

Here, $\vec{k}, \vec{k}'$ are electron momenta, $\sigma, \sigma'$ their spin directions and $\vec{w}$ phonon momenta, these are the quasi particles corresponding to the lattice oscillations. $v_{\vec{k}, \vec{k}', \vec{w}}$ gives the electron interaction induced by the interactions of the electrons and phonons, i.e. an electron with momentum $\vec{k}' + \vec{w}$ gives the momentum $\vec{w}$ to the lattice, which is taken by an electron with momentum $\vec{k}$. The spin is not changed by this interaction. With (real) coefficients $u_{\vec{k}}$ and $v_{\vec{k}}$ that will be arranged − taking care of the normalization $|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1$ − such that the energy expectation value of $|\Phi\rangle$ becomes minimal at the end of the day, the BCS ansatz for $|\Phi\rangle$ reads:

$$|\Phi\rangle = \prod_{\vec{k}} (u_{\vec{k}} + v_{\vec{k}} a_{\vec{k}, \downarrow}^+ a_{\vec{k}, \uparrow}) |0\rangle.$$ 

(1) Show $\langle \Phi | N | \Phi \rangle = 2 \sum_{\vec{k}} v_{\vec{k}}^2$ for the expectation value of the particle number operator. Since we want a fixed particle number, we have to add $N$ to $H$ using a Lagrange multiplier, the chemical potential $\mu$, i.e. $H' = H - \mu N$. 
(2) Using \( V_{kk'} = \frac{v_{kk} - v_{kk'}}{2} \), show that
\[
E_0 := \langle \Phi | H' | \Phi \rangle = 2 \sum \frac{(\varepsilon(\vec{k}) - \mu)}{v_{kk}^2} - \sum \frac{V_{kk'}u_{kk}v_{kk'}}{v_{kk'}},
\]
In order to understand this gap better, we consider the quasi particles of this system.
(3) Show: with the gap \( \Delta_{\vec{k}} = \sum \frac{V_{kk'}u_{kk}v_{kk'}}{v_{kk'}} \) the condition for a minimum of (2) is:
\[
\left\{ \frac{u_{kk}^2}{v_{kk}} \right\} = \frac{1}{2} \left( 1 \pm \frac{\varepsilon(\vec{k}) - \mu}{\sqrt{(\varepsilon(\vec{k}) - \mu)^2 + \Delta_{\vec{k}}^2}} \right).
\]
In order to understand this gap better, we consider the quasi particles of this system.
(4) Show that the ansatz \( | \Phi \rangle \) for the ground state is annihilated by the operators
\[
A(\vec{k}) = u_{kk}a_{\vec{k},1} - v_{kk}a_{\vec{k},1}^+, \quad B(\vec{k}) = u_{kk}a_{\vec{k},1} + v_{kk}a_{\vec{k},1}^+
\]
(5) Show that the only nonvanishing anticommutation relations of the operators defined in (4) are \( \{ A(\vec{k}), A^+(\vec{k}') \} = \{ B(\vec{k}), B^+(\vec{k}') \} = \delta_{\vec{k}\vec{k}'} \).
(6) Show that \( H' - E_0 \mathbb{1} \) is diagonal in the one-quasiparticle states \( A^+(\vec{k})| \Phi \rangle \) and \( B^+(\vec{k})| \Phi \rangle \) and that \( E(\vec{k}) = \sqrt{(\varepsilon(\vec{k}) - \mu)^2 + \Delta_{\vec{k}}^2} \) is the quasiparticle energy:
\[
\langle \Phi | A(\vec{k}) (H' - E_0 \mathbb{1}) A^+(\vec{k}') | \Phi \rangle = \langle \Phi | B(\vec{k}) (H' - E_0 \mathbb{1}) B^+(\vec{k}') | \Phi \rangle = E(\vec{k})\delta_{\vec{k}\vec{k}'}
\]
i.e. the quasiparticles have a nonvanishing energy \( \Delta_{\vec{k}} \) even for \( \vec{k} \) at the Fermi edge (which corresponds to a free particle at rest).
(7) Show that (3) is equivalent to \( \Delta_{\vec{k}} = \left\{ \frac{\Delta_{\vec{k}}}{\sqrt{(\varepsilon(\vec{k}) - \mu)^2 + \Delta_{\vec{k}}^2}} \right\} \).
(8) Take the ansatz \( V_{kk'} = V_0 \) for \( |\varepsilon(\vec{k}) - \mu| < \hbar \omega \) and \( |\varepsilon(\vec{k}') - \mu| < \hbar \omega \), in all other cases zero, i.e. the interaction only takes place in the neighbourhood of the Fermi sphere (radius=\( E_F = \mu \)). Deduce that \( \sum_{\vec{k}} \frac{1}{2\sqrt{(\varepsilon(\vec{k}) - \mu)^2 + \Delta_{\vec{k}}^2}} = \frac{1}{V_0} \), where \( \Delta \) is the now \( \vec{k} \) independent value of \( \Delta_{\vec{k}} \) for \( |\varepsilon(\vec{k}) - \mu| < \hbar \omega \), otherwise one has \( \Delta_{\vec{k}} = 0 \).
(9) Replace the sum by an integral in (8). For that, take the ansatz \( d^3k = (2\pi)^3 D(E - \mu) d(E - \mu) \). with the density of states \( D(E - \mu) \). Assume that \( \hbar \omega \ll \mu \), i.e. \( D(E - \mu) \approx D(0) \) and deduce \( \Delta = \frac{\hbar \omega}{\sinh(\hbar \omega/2D(0)V_0)} \approx 2\hbar \omega e^{-1/D(0)V_0} \) for \( D(0)V_0 < 1 \).
(10) Show that the electron interaction actually lowers the energy by \( \frac{1}{2} D(0)\Delta^2 \) compared to a filled Fermi sphere (assume \( \Delta \ll \hbar \omega \)).

(24 points)

H8.2 Squeezed States

(1) By deriving with respect to \( \alpha \), show that \( \langle e^{\alpha x} f \rangle = f(e^{\alpha} x) \) for \( f : \mathbb{R} \to \mathbb{C} \).
(2) For a one dimensional harmonic oscillator, consider the normalised state \( |\psi_\alpha\rangle = C_\alpha e^{\frac{\alpha}{2}((a^+)^2 - a^2 - 1)}|\varphi\rangle \) where \( \varphi \in L^2(\mathbb{R}) \). Use (1) and the explicit representation of \( a \) and \( a^+ \) in position space in order to represent \( \psi_\alpha(x) \) by \( \varphi(x') \), i.e. find the relation \( x'(x) \). Why is \( |\psi_\alpha\rangle \) called squeezed?
(3) Show that \( S := e^{x(a^+)^2 - x^2a^2} \) for \( z \in \mathbb{C} \) is unitary. How does that effect \( C_\alpha \)?

(6 points)