Exercises VIII

December 10th

E8.1 *Foundations of statistical physics, Bose–Einstein condensation*
Particle with Spin S confined to a box $B = \{\vec{r} \in \mathbb{R}^3 \,|\, 0 \le x_k \le L\}$ with length L and volume $V = L^3$ have wave functions ($\chi^{(\sigma)}$ a spinor):

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

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

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

Z is called *partition function*, μ *chemical potential* and with the *temperature* T and *Boltzmann's constant* k one has $\beta = \frac{1}{kT}$. The two "Lagrange multipliers" μ and β adjust the particle number and the energy. μ 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 $\langle\mathcal{O}\rangle := \mathrm{Tr}(\mathcal{O}\varrho)$.
In H7.2 we had: $Z = \prod_{\vec{n}} (1 \pm \mathrm{e}^{-\beta(\varepsilon(\vec{n})-\mu)})^{\pm g}$, $g = 2S+1$ and $\langle n_{\vec{n},\sigma}\rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon(\vec{n})-\mu)} \pm 1}$ for the average occupation of the state $(\vec{n},\sigma)$, where "+" is taken for fermions. We define the mean particle number $\overline{N} = \sum_{\vec{n},\sigma}\langle n_{\vec{n},\sigma}\rangle$ and energy $\overline{E} = \sum_{\vec{n},\sigma} \varepsilon(\vec{n})\langle n_{\vec{n},\sigma}\rangle$.

(1) Why is $\mu \le 0$ for bosons? Is there a restriction on μ in the fermionic case?

(2) Establish the replacement $\sum_{\vec{n},\sigma} \to g\frac{V}{(2\pi\hbar)^3}\int \mathrm{d}^3p$ in the continuum limit $V \to \infty$. Show that the limits for $V \to \infty$ of $\frac{\overline{E}}{V}$, $\frac{\overline{N}}{V}$ and $\frac{\ln Z}{V}$ do exist and compute them for $\varepsilon(\vec{p}) = \frac{1}{2m}\vec{p}^2$. Introduce the Fermi and Bose functions

$$\left\{\begin{matrix} f_\nu(z) \\ g_\nu(z) \end{matrix}\right\} = \frac{1}{\Gamma(\nu)}\int_0^\infty \frac{\mathrm{d}x\, x^{\nu-1}}{\frac{1}{z}\mathrm{e}^x \pm 1}.$$

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

(3) Show $\overline{E} = \frac{3}{2\beta}\ln Z$ and compute the classical limit, defined in such a way that $z := \mathrm{e}^{\mu/kT} \ll 1$. z is called *fugacity*. State this condition in the form $\lambda^3 \ll \frac{V}{\overline{N}}$ 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 $\Phi = -pV$. $p := -\frac{\partial\overline{E}}{\partial V}$ is the pressure. For that purpose show $p = \frac{2\overline{E}}{3V}$, before taking $V \to \infty$.

(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 $\overline{N} = \frac{gV|\vec{p}_F|^3}{6\pi^2\hbar^3}$ and deduce $\overline{E} = \frac{3}{5}E_F\overline{N}$. Argue that $\mu = E_F$.

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 $\frac{\lambda^3 \overline{N}}{V} = g_{3/2}(z)$.

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

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

(8) By considering the ground state separately, show that

$$\overline{N} = N_0 + N' = \frac{1}{\frac{1}{z} - 1} + \overline{N}\left(\frac{T}{T_c}\right)^{3/2} \frac{g_{3/2}(z)}{g_{3/2}(1)}.$$

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

$$\lim_{\overline{N}\to\infty,\ \frac{\overline{N}}{V}\ \text{fest}} \frac{N_0}{\overline{N}} \begin{cases} = 0 & T > T_c \\ > 0 & T < T_c \end{cases} \qquad (\text{“thermodynamic limit”}).$$

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.

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

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

Here, $\vec{k}, \vec{k}'$ are electron momenta, σ, σ' 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:

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

(1) Show $\langle\Phi|N|\Phi\rangle = 2\sum_{\vec{k}} v^2_{\vec{k}}$ 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 μ, i.e. $H' = H - \mu N$.

(2) Using $V_{\vec{k}\vec{k}'} = \frac{v_{\vec{k},-\vec{k}',\vec{k}'-\vec{k}}+v_{-\vec{k},\vec{k}',\vec{k}-\vec{k}'}}{2}$, show that

$$E_0 := \langle\Phi|H'|\Phi\rangle = 2\sum_{\vec{k}}(\varepsilon(\vec{k})-\mu)v_{\vec{k}}^2 - \sum_{\vec{k},\vec{k}'} V_{\vec{k}\vec{k}'}u_{\vec{k}}v_{\vec{k}}u_{\vec{k}'}v_{\vec{k}'}.$$

(3) Show: with the *gap* $\Delta_{\vec{k}} = \sum_{\vec{k}'} V_{\vec{k}\vec{k}'}u_{\vec{k}'}v_{\vec{k}'}$ the condition for a minimum of (2) is:

$$\begin{Bmatrix} u_{\vec{k}}^2 \\ v_{\vec{k}}^2 \end{Bmatrix} = \frac{1}{2}\left(1 \pm \frac{\varepsilon(\vec{k})-\mu}{\sqrt{(\varepsilon(\vec{k})-\mu)^2+\Delta_{\vec{k}}^2}}\right).$$

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

$$A(\vec{k}) = u_{\vec{k}}a_{\vec{k},\uparrow} - v_{\vec{k}}a^+_{-\vec{k},\downarrow}, \quad B(\vec{k}) = u_{\vec{k}}a_{-\vec{k},\downarrow} + v_{\vec{k}}a^+_{\vec{k},\uparrow}$$

(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).

But now back to the determination of $\Delta_{\vec{k}}$, for which we make use of a simple model.

(7) Show that (3) is equivalent to $\Delta_{\vec{k}} = \frac{1}{2}\sum_{\vec{k}'} \frac{V_{\vec{k}\vec{k}'}\Delta_{\vec{k}'}}{\sqrt{(\varepsilon(\vec{k}')-\mu)^2+\Delta_{\vec{k}'}^2}}$.

(8) Take the ansatz $V_{\vec{k}\vec{k}'} = V_0$ 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=μ). Deduce that $\sum_{\vec{k}} \frac{1}{2\sqrt{(\varepsilon(\vec{k})-\mu)^2+\Delta^2}} = \frac{1}{V_0}$, where Δ 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 $\mathrm{d}^3k = \frac{(2\pi)^3}{V}D(E-\mu)\mathrm{d}(E-\mu)$. with the density of states $D(E-\mu)$. Assume that $\hbar\omega \ll \mu$, i.e. $D(E-\mu) \approx D(0)$ and deduce $\Delta = \frac{\hbar\omega}{\sinh(\frac{1}{D(0)V_0})} \approx 2\hbar\omega \mathrm{e}^{-1/D(0)V_0}$ for $D(0)V_0 \ll 1$.

(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 α, show that $(\mathrm{e}^{\alpha x \frac{\partial}{\partial x}} f)(x) = f(\mathrm{e}^{\alpha}x)$ for $f: \mathbb{R} \to \mathbb{C}$.

(2) For a one dimensional harmonic oscillator, consider the normalised state $|\psi_\alpha\rangle = C_\alpha \mathrm{e}^{\frac{\alpha}{2}((a^+)^2 - a^2 - 1)}|\varphi\rangle$i where $\varphi \in \mathcal{L}^2(\mathbb{R})$. 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 squezzed?

(3) Show that $S := \mathrm{e}^{z(a^+)^2 - z^* a^2}$ for $z \in \mathbb{C}$ is unitary. How does that effect C_α?

(6 points)