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Problem Set 7

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Exercise 1 : Paramagnetism (quantum approach)

We consider a system of N atoms, each of which has a total angular momentum $\vec{J} = \vec{S} + \vec{L}$, in units of $\hbar$, with an absolute square value $\vec{J}^2 = J(J+1)$, where J is the quantum number of the total angular momentum. The magnetic moment of the atom n is $\vec{\mu}_n = -g\mu_B \vec{J}_n$, where g is the Landé factor of the considered atoms.

a) Write the Hamiltonian describing the Zeeman energy of the atoms with an applied magnetic field $\vec{B}$ parallel to the z-axis for a N-atom system. Specify the possible values J_n^z of the projection of the angular momentum $\vec{J}$ of atom n on the z-axis.

$$H_z = -\sum_i \vec{\mu}_i \cdot \vec{B}$$

$$\vec{\mu}_i = -g\mu_B \vec{J}_i$$

Thus,

$$H_z = g\mu_B \sum_i \vec{B} \cdot \vec{J}_i$$

$$J^z \in \{-j, -j+1, \cdots, j-1, j\}$$

Thus,

$$H_z = g\mu_B \sum_i B J_i^z$$

b) The atoms are supposed to be independent. Write the partition function Z of the system. Show that it can be expressed as a function of the ratio of two hyperbolic sines $\sinh A_1 / \sinh A_2$, and determine A_1 and A_2.

$$\begin{aligned} Z &= \sum_{\{J_i^z\}} \sum_{J^z} e^{-\beta g \mu_B \sum_i B J^z} \\ &= \left(\sum_{J^z} \left[e^{-\beta g \mu_B J^z B} \right] \right)^N \\ &= z^N \end{aligned}$$

$$
\begin{aligned}
z &= \sum_{J^z} e^{-\beta g \mu_B B J^z} \\
&= \sum_{J^z} \left(e^{-\beta g \mu_B B}\right)^{J^z} \qquad\qquad K = J^z + j \\
&= \sum_{K=0}^{2j} \left(e^{-\beta g \mu_B B}\right)^{K-j} \\
&= e^{\beta g \mu_B B j} \sum_{K=0}^{2j} \left(e^{-\beta g \mu_B B}\right)^{K} \\
&= e^{\beta g \mu_B B j} \left(\frac{1 - e^{-\beta g \mu_B B (2j+1)}}{1 - e^{-\beta g \mu_B B}}\right) \\
&= \frac{\sinh(\beta g \mu_B B (j + 1/2))}{\sinh(\beta g \mu_B B/2)}
\end{aligned}
$$

$$
Z = \left(\frac{\sinh(\beta g \mu_B B (j + 1/2))}{\sinh(\beta g \mu_B B/2)}\right)^N
$$

c) The free energy of the system is $F = -k_B T \ln(Z)$. We denote E_l the energy of the N-atom system in a microscopic state l. In this state, each atom n has a magnetic moment $\vec{\mu}_n^l$. Express E_l as a function of the applied magnetic field $\vec{B}$ and the total magnetic moment $\vec{m}_l$ of the system, and show that the mean value of the magnetic moment is given by $\langle m \rangle = -\partial F / \partial B$.

d) Show that the magnetization M defined as the mean magnetic moment per unit volume can be expressed as $M = D \times B_J(X)$, where

$$
B_J(X) = \frac{2J+1}{2J} \coth\left[\frac{2J+1}{2J} X\right] - \frac{1}{2J} \coth\left[\frac{1}{2J} X\right]
$$

denotes the Brillouin function. Determine D and X.

$$
\begin{aligned}
F &= -k_B T \ln Z \\
&= -N k_B T \ln(z)
\end{aligned}
$$

$$
\begin{aligned}
M &= \frac{\langle m \rangle}{V} \\
&= -\frac{1}{V} \frac{\partial F}{\partial B} \\
&= n k_B T \frac{\partial \ln(z)}{\partial B} \\
&= n k_B T \frac{\left(\frac{\partial z}{\partial B}\right)}{z}
\end{aligned}
$$

Let's assume $x = \beta g \mu_B B$,

$$\frac{\partial z}{\partial B} = \frac{\beta g \mu_B (j+1)\cosh(x(j+1/2))\sinh(x/2) - \frac{1}{2}\beta g \mu_B \sinh(x(j+1/2))\cosh(x/2)}{\sinh(x/2)^2}$$

Let's assume $X = j\beta g \mu_B B$,

$$\begin{aligned} M &= n g \mu_B \left[(j+1/2)\coth(x(j+1)) - \frac{1}{2}\coth(x/2) \right] \\ &= n g \mu_B j \left[\frac{j+\frac{1}{2}}{j}\coth\left(\frac{X(j+1/2)}{j}\right) - \frac{1}{2j}\coth(X/2j) \right] \\ &= D \times B_J(X) \end{aligned}$$

$$D = n g \mu_B j$$

e) Deduce the value of the high-temperature susceptibility when $X \ll 1$. Is the system paramagnetic ?

$$\coth(x) \approx \frac{1}{x} + \frac{x}{3} + \cdots$$

$$\begin{aligned} M &= D \times \left(\frac{2j+1}{2j}\left(\frac{2j}{(2j+1)X} + \frac{2j+1}{6j}X \right) - \frac{1}{2j}\frac{2j}{X} - \frac{1}{2j}\frac{X}{6j} \right) \\ &= D \times \left(\frac{1}{X} + \frac{(2j+1)^2}{12J^2}X - \frac{1}{X} - \frac{X}{12j^2} \right) \\ &= D \times \frac{X}{3}\frac{j(j+1)}{j^2} \\ &= \frac{n g \mu_B}{3}(j+1)X \end{aligned}$$

$$\chi = \frac{n g \mu_B}{3}(j+1)\beta g \mu_B j = \frac{n g^2 \mu_B^2 j(j+1)}{3 k_B T}$$

For $X \gg 1$,

$$M = n g \mu_B j = n\mu$$

Yes the system is paramagnetic.

Exercise 2 : Landau levels

We study a two-dimensional electron gas in an external magnetic field $\vec{B} = B\vec{e}_z$ oriented along the z-axis. We do not take into account the spin, and consider electrons as particles with charge $-e$ and mass m.

a) Write the classical equation of motion for an electron in the x—y plane and show that the solutions are circular orbits. Calculate the angular velocity ω_c (the cyclotron frequency) and the radius r_c of the classical motion in these orbits.

Cyclotron frequency

$$\omega_c = \frac{eB}{m}$$

Radius,

$$r_c = \frac{|\vec{v}|}{\omega_c}$$

b) Use the Landau gauge $\vec{A} = A_x\vec{e}_x$ for the vector potential. Determine A_x and write the time-independent Schrödinger equation for an electron in the x^-y plane.

$$\vec{A} = \begin{pmatrix} -By \\ 0 \\ 0 \end{pmatrix}$$

And thus,

$$\frac{1}{2m}\left(\vec{p} - e\vec{A}\right)^2 \psi(x, y) = E\psi(x, y)$$

c) Use the product ansatz $\psi_{n,k}(x, y) = \varphi_n^{(k)}(y)e^{ikx}$ to relate the Schrödinger equation to the harmonic oscillator problem. Express $\varphi_n^{(k)}(y)$ in terms of shifted harmonic oscillator eigenfunctions. Show that the corresponding energy levels are given by $\epsilon_n = \hbar\omega_c(n + 1/2)$ and independent of k. Such levels are called Landau levels. What is the group velocity corresponding to the plane-wave component in x-direction ?

Product Ansatz,

$$\psi(x, y) = e^{ikx}\varphi_n^{(k)}(y)$$

And thus,

$$\left[\frac{p_y^2}{2m} + \frac{m\omega_c^2}{2}(y + y_k)^2\right]\varphi_n^{(k)}(y) = E_n\varphi_n^{(k)}(y) \qquad y_k = \frac{\hbar k}{eB}$$

Which is simply an harmonic oscillator shifted in the y direction, centered on $y = y_k$, with the energies,

$$E_n = \hbar\omega_c \left(n + \frac{1}{2}\right)$$

$$\varphi_n^{(k)}(y) = \varphi_n^{\mathrm{HO}}(y + y_k)$$

Group velocity,

$$v_g = \frac{1}{\hbar}\frac{\partial E}{\partial k} = 0$$

So, an electron in one of these states will not move.

d) Consider a rectangular system of size $L_x \times L_y$ with periodic boundary conditions. Discuss the allowed values for k and calculate the degeneracy of the Landau levels as a function of the cyclotron frequency. Give a physical interpretation of the degeneracy.

$$e^{ikx} = e^{ik(x+L_x)} \longrightarrow k = \frac{2\pi}{L_x} n_x, \qquad n_x \in \mathbb{Z}$$

$$0 \leq -y_k \leq L_y \longrightarrow 0 \leq -\frac{\hbar}{eB}\frac{2\pi}{L_x} n_x \leq L_y \longrightarrow n_x \geq -\frac{eBL_x \times L_y}{2\pi\hbar} \geq 0$$

And so we have,

$$n_x \in \left[-\frac{eBL_x \times L_y}{h}, 0\right]$$

$g_{\mathrm{LL}} =$ the number of $n_x = eBL_x \times L_y/h = m\omega_c L_x \times L_y/h$.
This degeneracy is the same for all the levels.

e) Calculate the magnetic flux through the system and express it in units of the flux quantum $\phi_0 = h/e$. Comment the result in the context of the degeneracy of the Landau levels.

$$\Phi = BL_x \times L_y \longrightarrow \frac{\Phi}{\Phi_0} = \frac{eBS}{h} = g_{\mathrm{LL}}$$

Each state correspond to a value of flux quantum.

f) Compare the average density of states to the density of states in the absence of a magnetic field.

SCHEMA

$$\rho(E) = \frac{g_{\rm LL}}{L_x \times L_y} \sum_n \delta(E - E_n)$$

$$\langle \rho(E) \rangle = \frac{g_{\rm LL}}{L_x \times L_y} \frac{1}{\Delta E} = \frac{m\omega_c L_x \times L_y}{h L_x \times L_y} \frac{1}{\hbar\omega_c} = \frac{2\pi m}{\hbar^2}$$

Which is exactly the density of states of 2D.

Exercise 3 : Landau diamagnetism

We now consider electrons in three dimensions in an external magnetic field $\vec{B} = B\vec{e}_z$ oriented along the z-axis, and continue to ignore the spin degree of freedom.

a) Extend the product ansatz of Exercise 2 towards the three-dimensional case in a large rectangular cuboid of size $L_x \times L_y \times L_z$ and show that, when $B \neq 0$, the energy of an electron depends on the quantum number n and on the wave-number in z-direction k_z as

$$\epsilon_{n,k_z} = \hbar\omega_c \left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m},$$

where $\omega_c = eB/m$ is the cyclotron frequency. Discuss the result.

$$\psi(x, y, z) = e^{ik_z z}\psi_{\mathrm{LL}}(x, y)$$

$$H_{xy}\psi_{\mathrm{LL}} = \hbar\omega_c(n + 1/2)\psi_{\mathrm{LL}}$$

$$\left(H_{xy} - \frac{\hbar^2\partial_z^2}{2m}\right)\psi = \left(\hbar\omega_c(n + 1/2) + \frac{\hbar^2 k_z^2}{2m}\right)\psi$$

b) The problem will be treated within the grand canonical ensemble. Write the grand partition function $\mathcal{Z} = \sum \exp[(\mu N - E)/k_B T]$ as a sum over many-body microstates characterized by the total particle number N and energy E. Show that in the case of non-interacting fermions one can write the grand potential $\Omega = -k_B T \ln Z$ in the form

$$\Omega = -k_B T \sum_s \ln\left[1 + e^{(\mu - \epsilon_s)/k_B T}\right]$$

as a sum over one-body states s.

$$\mathcal{Z} = \sum \exp(\beta(\mu N - E))$$

$$\begin{aligned}
\Omega &= -k_B T \ln(\mathcal{Z}) \\
&= -k_B T \ln\left(\sum_{\{n_s\}} \exp\left(\beta(\mu \sum_s n_s - \sum_s \varepsilon_s n_s)\right)\right) \\
&= -k_B T \sum_s \ln\left(1 + e^{\beta(\mu - \epsilon_s)}\right)
\end{aligned}$$

c) Write the grand potential as sum over the Landau level index n and the momentum in z-direction p_z. Replace the sum over p_z by an integral and show that Ω can be written as

$$\Omega = \hbar\omega_c \sum_{n=0}^{\infty} f(\mu - \hbar\omega_c[n+1/2])$$

Determine the function $f(x)$.

$$\begin{aligned}\Omega &= -k_B T \sum_s \ln\left(1 + e^{\beta(\mu-\epsilon_s)}\right) \\ &= -k_B T \sum_{n,p} \ln\left(1 + e^{\beta(\mu-\hbar\omega_c(n+1/2)+p_z^2/2m)}\right) \times g_{\mathrm{LL}} \\ &= -k_B T g_{\mathrm{LL}} \sum_n \sum_p \ln\left(1 + e^{\beta(\mu-\hbar\omega_c(n+1/2)+p_z^2/2m)}\right)\end{aligned}$$

$$e^{ik_z z} = e^{ik_z(z+L_z)} \longrightarrow k_z = \frac{2\pi N}{L_z} \rightarrow \Delta p_z = \frac{h}{L_z}$$

$$\begin{aligned}\Omega &\simeq -k_B T g_{\mathrm{LL}} \sum_n \int \mathrm{d}p \frac{L_z}{h} \ln\left(1 + e^{\beta(\mu-\hbar\omega_c(n+1/2)} e^{-\beta p^2/2m}\right) \\ &= \hbar\omega_c \sum_{n=0}^{\infty} \underbrace{\left(\frac{-2\pi k_B T V m}{h^3}\right) \int \mathrm{d}p \ln\left(1 + e^{\beta x} e^{-\beta p^2/2m}\right)}_{f(x)}\end{aligned}$$

d) Apply the variant of the Euler-MacLaurin formula

$$\sum_{n=0}^{\infty} F(n+1/2) \approx \int_0^{\infty} \mathrm{d}x F(x) + \frac{1}{24} F'(0)$$

to the sum over n. In which limit is this formula a good approximation? Show that the result can be expressed as

$$\Omega = \Omega_0(\mu) - \frac{(\hbar\omega_c)^2}{24} \frac{\partial^2 \Omega_0(\mu)}{\partial \mu^2},$$

with Ω_0 the grand potential in the absence of a magnetic field.

This is a good approximation when $\beta\hbar\omega_c \ll 1$ so it's a small magnetic field or high temperature limit.

$$F(x) = f(\mu - \hbar\omega_c x)$$

$$\Omega = \hbar\omega_c \sum_n F(n+1/2)$$
$$\approx \int_0^{+\infty} \mathrm{d}x F(x) + \frac{1}{24} F'(0)$$
$$= \Omega_0(\mu) - \frac{(\hbar\omega_c)^2}{24} f'(\mu)$$

$$\Omega = \underbrace{\hbar\omega_c \int_0^{+\infty} \mathrm{d}x f(\mu - \hbar\omega_c x)}_{\Omega_0(\mu)} + \frac{1}{24}\hbar\omega_c \frac{\partial}{\partial x} f(\mu - \hbar\omega_c x)\Big|_{x=0}$$

Let's calculate $\Omega_0(\mu)$,

$$\Omega_0 = \hbar\omega_c \int_0^{+\infty} \mathrm{d}x f(\mu - \hbar\omega_c x) \qquad y = \mu - \hbar\omega_c x$$
$$= \int_{-\infty}^{\mu} \mathrm{d}y f(y)$$

So there is no dependence on the magnetic field for $\Omega_0(\mu)$.

$$\frac{1}{24}\hbar\omega_c \frac{\partial}{\partial x} f(\mu - \hbar\omega_c x)\Big|_{x=0} = -\frac{1}{24}(\hbar\omega_c)^2 \frac{\partial}{\partial y} f(y)\Big|_{y=\mu}$$
$$= -\frac{1}{24}(\hbar\omega_c)^2 \frac{\partial^2}{\partial\mu^2}\Omega_0(\mu)$$

$$\Omega = \Omega_0(\mu) - \frac{(\hbar\omega_c)^2}{24} \frac{\partial^2\Omega_0(\mu)}{\partial\mu^2}$$

e) Use the result for Ω to relate the magnetic susceptibility per volume $\chi = -\frac{\mu_0}{V}\frac{\partial^2\Omega}{\partial B^2}$ to the density of states at the chemical potential $\rho(\mu)$. Show that the resulting Landau susceptibility for electrons with spin corresponds to diamagnetic behavior and is given by $\chi_{\text{Landau}} = -\chi_{\text{Pauli}}/3$, where $\chi_{\text{Pauli}} = \mu_0\mu_B^2\rho(\mu)$ is the paramagnetic Pauli susceptibility (which is due to the spins of the electrons).

$$-\frac{\mu_0}{V}\frac{\partial\Omega}{\partial B} = M = \frac{2\mu_0}{V}\frac{\partial^2\Omega_0}{\partial\mu^2}\frac{\hbar^2 e^2}{24m^2} B = \chi_m B$$

And so,

$$\chi_m = \frac{\mu_0\hbar^2 e^2}{12Vm^2}\frac{\partial^2\Omega_0}{\partial\mu^2}$$
$$= \frac{\mu_0}{3}\frac{\mu_B^2}{V}\frac{\partial^2\Omega_0}{\partial\mu^2}$$

$$\frac{1}{V}\frac{\partial\Omega}{\partial\mu} = -\frac{1}{V}\frac{k_BT}{Z}\frac{\partial Z}{\partial\mu} = -n$$

$$\frac{1}{V}\frac{\partial^2\Omega_0}{\partial\mu^2} = -\frac{\partial n}{\partial\mu} = -\rho(\mu)$$

$$n = \int_{-\infty}^{\mu} \mathrm{d}E\rho(E)$$

And so,

$$\chi_m = -\frac{1}{3}\mu_B^2\rho(\mu)\mu_0 = -\frac{1}{3}\chi_{\text{Pauli}}$$