Exam — Session 1

Duration: 2 h

Documents, cell phones, computers, tablets, pocket calculators, etc., are not allowed

The text contains 3 pages in total

1 Degenerate electron gas

Let us consider a gas of noninteracting electrons with mass m confined in a square box of volume $V = L^3$, with L the length of the sides. The gas is maintained at a fixed temperature T and chemical potential μ (grand-canonical ensemble).

We recall that electrons are spin 1/2 particles, so that they obey the Fermi–Dirac statistics. The average occupancy of a quantum state λ with energy ε_λ is then given by the Fermi–Dirac distribution

$$f(\varepsilon_\lambda) = \frac{1}{\mathrm{e}^{\beta(\varepsilon_\lambda - \mu)} + 1}, \tag{1.1}$$

where $\beta = 1/k_\mathrm{B}T$.

1.1 General results for noninteracting fermions

(a) Plot the Fermi–Dirac distribution (1.1) as a function of the single-particle energy ε_λ for (i) $T = 0$ and (ii) $T \neq 0$. At $T = 0$, how is called the energy of the highest occupied level?

(b) Carefully demonstrate that the grand-canonical partition function for noninteracting fermions is given by

$$\Xi = \prod_\lambda \left[1 + \mathrm{e}^{-\beta(\varepsilon_\lambda - \mu)}\right],$$

where the product runs over quantum states λ with energy ε_λ.

(c) Deduce from the previous result that the general expression of the grand potential for noninteracting fermionic particles is given by

$$\Omega = -k_\mathrm{B}T \sum_\lambda \ln\left(1 + \mathrm{e}^{-\beta(\varepsilon_\lambda - \mu)}\right). \tag{1.2}$$

1.2 Nonrelativistic electrons

We now consider that the electrons are nonrelativistic. Their possible energy levels are given (using periodic boundary conditions) by

$$\varepsilon_\mathbf{k} = \frac{\hbar^2|\mathbf{k}|^2}{2m}, \qquad \mathbf{k} = \frac{2\pi}{L}(n_x, n_y, n_z),$$

where the three quantum numbers $n_x, n_y, n_z \in \mathbb{Z}$.

(a) Show that the density of states $\rho(\varepsilon)$ is given in the thermodynamic limit by

$$\rho(\varepsilon) = KV\sqrt{\varepsilon},$$

where K is a constant. Give the expression of K as a function of m and $\hbar$.

(b) Show that the average energy of the system is given by

$$E = KV \int_0^\infty \mathrm{d}\varepsilon \, \frac{\varepsilon^{3/2}}{\mathrm{e}^{\beta(\varepsilon - \mu)} + 1}. \tag{1.3}$$

(c) Using Eqs. (1.2) and (1.3), demonstrate that

$$\Omega = -\frac{2}{3}E.$$

(d) Deduce from the two previous questions that the pressure of the gas is given by

$$P = \frac{2E}{3V}.$$

(e) Demonstrate that the Fermi energy is given in terms of the electron density $n = N/V$ by

$$\varepsilon_{\mathrm{F}} = \left(\frac{3n}{2K}\right)^{2/3}.$$

Hint: Calculate first the average number of particles N at $T = 0$.

(f) Deduce from the above considerations that the pressure at $T = 0$ is given by

$$P = \frac{2(2\pi^2)^{2/3}}{15}\frac{\hbar^2}{m}\left(\frac{3n}{2}\right)^{5/3}.$$

What is the physical interperation of this result? How does it compare to the pressure in the nondegenerate limit?

2 Ising model with long-range interactions

We consider a system of $N \gg 1$ spins $s_i = \pm 1$ on a square lattice in dimension d at the temperature T. In the Ising model with long-range interactions, each spin interacts with all the other spins of the lattice with the same interaction energy. The Hamiltonian of the model reads

$$\mathcal{H} = -\frac{J}{2N}\sum_{\substack{i,j=1 \\ (i\neq j)}}^{N} s_i s_j - h\sum_{i=1}^{N} s_i, \tag{2.1}$$

where $J > 0$ is the coupling constant and $h > 0$ is the external magnetic field. In what follows, we denote $\beta = 1/k_{\mathrm{B}}T$, with k_{B} the Boltzmann constant.

2.1 Warm up

(a) What do the different terms of the Hamiltonian correspond to?

(b) What is the ground state of the model? Calculate the average energy of this state. Why is it important to normalize the interaction term by $1/N$?

(c) Show that it is possible to rewrite the Hamiltonian (2.1) as

$$\mathcal{H} = \frac{J}{2} - \frac{J}{2N}\left(\sum_{i=1}^{N} s_i\right)^2 - h\sum_{i=1}^{N} s_i.$$

2.2 Partition function and free energy

(a) Give the formal expression of the canonical partition function Z without trying to calculate it.

(b) Using the relation

$$\exp\left(\frac{1}{2}\alpha^2\right) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x \, \exp\left(-\frac{1}{2}x^2 + \alpha x\right),$$

show that is is possible to express the partition function as

$$Z = \exp\left(-\frac{\beta J}{2}\right) \sqrt{\frac{N\beta}{2\pi J}} \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon \, \exp\left[-N g\left(\varepsilon\right)\right], \tag{2.2}$$

with $\varepsilon = \sqrt{J/(N\beta)}\, x$ and

$$g(\varepsilon) = \frac{\beta}{2J}\varepsilon^2 - \ln\big(2\cosh\left(\beta[\varepsilon + h]\right)\big).$$

(c) We are now aiming at calculating the free energy per site of the system $f = F/N$ in the thermodynamic limit $N \gg 1$,

$$\beta f = -\lim_{N\to\infty} \frac{1}{N} \ln Z.$$

When $N \gg 1$, the integral in Eq. (2.2) can be calculated using the formula

$$\int_{-\infty}^{+\infty} \mathrm{d}\varepsilon \, \exp\big(-Ng(\varepsilon)\big) \underset{(N\gg 1)}{\simeq} \sqrt{\frac{2\pi}{N g''(\varepsilon_{\text{min}})}} \exp\big(-Ng(\varepsilon_{\text{min}})\big)$$

where ε_{min} is the value that minimizes the function $g(\varepsilon)$. Justify briefly this relation and show that in the thermodynamic limit $N \gg 1$

$$\beta f = \frac{\beta}{2J}\varepsilon_{\text{min}}^2 - \ln\big(2\cosh\left(\beta[\varepsilon_{\text{min}} + h]\right)\big), \tag{2.3}$$

with

$$\varepsilon_{\text{min}} = J \tanh\left(\beta[\varepsilon_{\text{min}} + h]\right).$$

(d) In the thermodynamic limit, is the expression (2.3) of βf an approximation or an exact result?

2.3 Equation of state and critical exponents

(a) Show that the average magnetization m is solution of the equation

$$m = \tanh\left(\beta[Jm + h]\right).$$

(b) Discuss the behavior of the system for $h = 0$ (nature of the transition, phase diagram, critical temperature T_c). A graphical discussion can be helpful.

(c) Calculate the critical exponents β, γ, and δ, defined as

$$\begin{aligned} &m \sim (T_\text{c} - T)^{\beta}, \qquad T \to T_\text{c}^-, \quad h = 0, \\ &m \sim h^{1/\delta}, \qquad T = T_\text{c}, \quad h \to 0, \\ &\chi = \left.\frac{\partial m}{\partial h}\right|_{(h=0)} \sim |T - T_\text{c}|^{-\gamma}, \qquad T \to T_\text{c}^{\pm}, \quad h = 0. \end{aligned}$$

Take special care of distinguishing between $T \to T_\text{c}^-$ and $T \to T_\text{c}^+$ when calculating γ.

2.4 Discussion

(a) Discuss briefly and qualitatively the mean-field approximation usually made to calculate the properties of the short-range Ising model.

(b) Explain why we can say that the mean-field approximation leads to an exact result in the long-range case.

(c) Does a phase transition exist in dimension $d = 1$ in this model with long-range interactions? How does it compare to the usual Ising model with short-range interactions?