Physics 727: Assignment 5

(to be submitted by Tuesday, April 30, 2024)

You may find it helpful to review §6.1, §6.2, §7.3, §7.4, §8.1, §8.2, §9.2, and §9.3 of Kennett's book.

1. A gas of ideal spinless fermions lives in a one-dimensional, periodic environment. The system is characterized by a length L and a repeat distance a. The dispersion relation connects each wave vector k (or momentum $p = \hbar k$) to a single-particle energy $\varepsilon_k = -2t \cos ka$. Here $t > 0$ is an energy scale related to the band width.

   (a) Argue that the grand partition function is

   $$\mathcal{Z} = \prod_k \left(1 + e^{-\beta(\varepsilon_k - \mu)}\right),$$

   where the product is over all allowed wave vectors

   $$\left\{ \frac{2\pi n}{N_\mathrm{u} a} = \frac{2\pi n}{L} : n = -\frac{N_\mathrm{u}}{2} + 1, \ldots, \frac{N_\mathrm{u}}{2} - 1, \frac{N_\mathrm{u}}{2} \right\}.$$

   Here, $N_\mathrm{u} = L/a$ is the (positive integer) number of unit cells.

   (b) If N_u is very large, we can assume a continuum of allowed wave vector values that form a Brioullin zone $k \in (-\pi/a, \pi/a]$. The wave vector spacing is $\Delta k = 2\pi/N_\mathrm{u} a = 2\pi/L \to dk$, and so we can let the k-vector sum pass over to an integral:

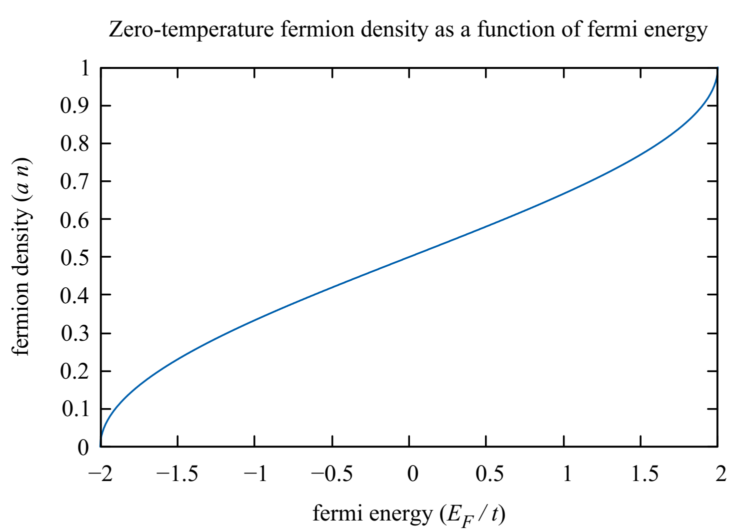
   $$\sum_k = \frac{1}{\Delta k} \sum_k \Delta k = \frac{L}{2\pi} \int dk.$$

   Provide an integral representation of the grand potential $\Phi(T, \mu) = -(1/\beta) \ln \mathcal{Z}$ in the continuum limit.

   (c) Show that the fermion density is

   $$n(T, \mu) = \frac{N}{L} = -\frac{1}{L} \frac{\partial \Phi}{\partial \mu} = \int \frac{dk}{2\pi} \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1}.$$

   (d) Compute n in the $T \to 0$ limit. Note that, at zero temperature, the chemical potential of a fermi gas is typically referred to as the fermi energy, $\mu = E_F$. Graph your result. You should be able to reproduce the following (which I created in `gnuplot`).



(e) Show that the compressibility of the fermion gas, $\partial n/\partial\mu$, has the following form at zero temperature:

$$\chi(E_F) = \lim_{\substack{T\to 0\\ \mu\to E_F}} \frac{\partial n}{\partial \mu} = \frac{1}{2\pi t a}\frac{1}{\sqrt{1-(E_F/2t)^2}}.$$

Explain that this is just the density of states, evaluated at the fermi energy. Show that the compressibility diverges as one over the square root of the fermi energy at the top ($E_F \to 2t$) and bottom ($E_F \to -2t$) of the energy band.

2. Consider a system of mass-m free bosons in three spatial dimensions, held at temperature $T = 1/k_B\beta$ and chemical potential μ. The corresponding grand potential is

$$\Phi = \frac{1}{\beta}\left[\ln\left(1-e^{\beta\mu}\right) + V\int \frac{d^3k}{(2\pi)^3}\ln\left(1-e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}\right)\right],$$

where $\varepsilon_{\mathbf{k}} = \hbar^2\mathbf{k}\cdot\mathbf{k}/2m = \hbar^2k^2/2m$ is the free-particle kinetic energy. Be sure to explain and justify the presence of the first term in the brackets.

(a) Compute the particle density N/V. Show that it can be massaged into the form

$$n(T,\mu) = \frac{N}{V} = \frac{1}{V}\frac{1}{e^{-\beta\mu}-1} + \frac{1}{4\pi^2}\left(\frac{2m}{\beta\hbar^2}\right)^{3/2} I_0(e^{\beta\mu}),$$

where

$$I_j(z) = \int_0^\infty \frac{x^{j+1/2}dx}{z^{-1}e^x - 1}.$$

(b) Plot $I_0(z)$, $I_1(z)$, and $I_2(z)$ on the interval $z\in[0,1]$. Observe that the functions are smooth, monotonically increasing, and bounded. Why have we focussed on this particular interval? What restrictions are there on the values of β and μ?

```
f[z_, j_] := Integrate[x^(j + 1/2)/((1/z)*Exp[x] - 1), {x, 0, \[Infinity]}]
mesh = Range[50]/50.
vals0 = f[#, 0]& @ mesh
vals1 = f[#, 1]& @ mesh
vals2 = f[#, 2]& @ mesh
data0 = Transpose[{mesh, vals0}]
data1 = Transpose[{mesh, vals1}]
data2 = Transpose[{mesh, vals2}]
ListPlot[{data0, data1, data2}, PlotLabels -> {0, 1, 2}]
Table[f[1, j], {j, 0, 2}]
N[%]
```

(c) Compute the energy density U/V. Express it in terms of $I_1(z)$.

(d) Imagine that a gas of bosons is held at fixed density $n = N/V$ at a temperature high enough that its lowest-energy state (the zero-momentum state with $\varepsilon_{\mathbf{0}} = 0$) is not macroscopically occupied; i.e.,

$$\frac{1}{V}\frac{1}{e^{-\beta\mu}-1} \to 0.$$

Think about what happens as the temperature is lowered up to the threshold where this term would start contributing. Identify a temperature below which the constraint

$$n(T,\mu) = \frac{1}{4\pi^2}\left(\frac{2m}{\beta\hbar^2}\right)^{3/2} I_0(e^{\beta\mu}),$$

which is used to determine μ in terms of the known n, can no longer be satisfied.