12. (Statistical Mechanics)

Consider a d-dimensional gas of spin-1/2 electrons (two spin states per electron). The gas is enclosed in a rectangular box whose sides have equal length L. Assume that the box is large enough such that the spectrum may b approximated by a continuum.

Define the surface area of the d-dimensional hypersphere of radius r as $S_d r^{d-1}$ (e.g. $S_2 = 2\pi$ and $S_3 = 4\pi$).

(a) Given electron density $\rho = N/L^d$, where N is the total number of electrons, calculate the Fermi wavevector k_F. Express your answer in terms of d, ρ, and S_d.

(b) Using the definition $E_F = \hbar^2 k_F^2/2m$, calculate the density of states per unit volume, ρ_E as a function of energy E. Express your answer in terms of ρ, d, and E_F.

Solution: *Solution by Jonah Hyman (jthyman@g.ucla.edu)*

This problem relies on some background knowledge about phase space and the density of states:

Phase space and density of states:
Consider a particle in d-dimensional space. The particle's state can be defined by its position $\mathbf{x} = (x_1, \ldots, x_d)$, its momentum $\mathbf{p} = (p_1, \ldots, p_d)$, and any internal degrees of freedom (e.g. spin). Assume that there are g possible internal states for the particle.
The position and momentum of the particle constitute a point in $2d$-dimensional phase space: $(x_1, \ldots, x_d, p_1, \ldots, p_d)$.
To solve problems, discretize phase space by dividing it into $2d$-dimensional boxes. The volume of each box is h^d, where h is Planck's constant (which has units of position times momentum). The number of boxes in a phase-space volume $d^d p\, d^d x$ is the total volume divided by the volume of each box, or $\frac{d^d p\, d^d x}{h^d}$. Each box has g possible states, corresponding to the internal degrees of freedom of the particle. Therefore, the number of possible states in a phase-space volume $d^d p\, d^d x$ is

$$\text{Number of possible states in a phase-space volume } d^d p\, d^d x = g\frac{d^d p\, d^d x}{h^d} \tag{377}$$

To find the density of states in terms of the wavenumber k or the energy E, change variables from p to k or E, typically using the relation for free particles $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$ and converting to spherical coordinates. Also, for free particles, you can replace $d^d x$ with V, the total volume since the wavenumber and energy does not depend on x. You can then extract your answer using the relation

$$g\frac{d^d p\, d^d x}{h^d} = \rho_k\, dk = \rho_E\, dE \tag{378}$$

Part (a) also relies on understanding the Fermi wavenumber:

Fermi momentum/wavenumber/energy:
For a set of N free fermions in a volume V, the ground state consists of filling up the lowest-energy states until we have used up all N fermions. (By the Pauli exclusion principle, we can only fill each state once.) Since $E = \frac{p^2}{2m}$ for free particles, this consists of filling up the momentum part of phase space in a spherically symmetric manner. The momentum radius of that sphere is the Fermi momentum p_F.
To find the Fermi momentum p_F, calculate the number of possible states in a phase-space volume that is a sphere of radius p_F in the momentum part of phase space, and that occupies a volume V in the position part of phase space. Then, set this number equal to the number of particles N. In other words, solve the following equation for p_F:

$$N = \int_{p \le p_F} g\frac{d^d p\, d^d x}{h^d} = g\frac{V}{h^d}\int_{p \le p_F} d^d p \tag{379}$$

Here, g is the number of internal states per particle.
From the Fermi momentum, we can derive the Fermi wavenumber and the Fermi energy using

$$p_F = \hbar k_F \quad \text{and} \quad E_F = \frac{p_F^2}{2m} = \frac{\hbar^2 k_F^2}{2m} \tag{380}$$

(a) The form of the electron density $\rho = N/L^d$ may seem a bit confusing. It just means the total number of electrons over the total volume, and it is a different quantity than the density of states. We will use it only at the end of the calculation.

Our starting point is the equation (379). Here, the volume is L^2, so we get

$$N = g\frac{V}{h^d}\int_{p\le p_F} d^dp = g\frac{L^d}{h^d}\int_{p\le p_F} d^dp$$

This integrand is spherically symmetric, so we can replace the integration measure d^dp with a single integration measure dp:

$$d^dp = (\text{Surface area of } d\text{-dimensional hypersphere}) \cdot p^{d-1}dp = S_d\, p^{d-1}\, dp \tag{381}$$

For example, $d^3p = S_3p^2dp = 4\pi p^2dp$.

This boils the integral down to

$$\begin{aligned} N &= g\frac{L^d}{h^d}\int_{p=0}^{p=p_F} S_d\, p^{d-1}dp \\ &= g\frac{L^d}{h^d}S_d\int_{p=0}^{p=p_F} p^{d-1}\, dp \\ &= g\frac{L^d}{h^d}S_d\left[\frac{p^d}{d}\right]_{p=0}^{p=p_F} \\ N &= g\frac{L^d}{h^d}S_d\frac{p_F^d}{d} \end{aligned} \tag{382}$$

Using the fact that $p_f = \hbar k_F$ and $h = 2\pi\hbar$, this simplifies to

$$N = g\frac{L^d}{d(2\pi\hbar)^d}S_d\left(\hbar k_F\right)^d = g\frac{L^d}{d(2\pi)^d}S_dk_F^d$$

We can now solve for k_F:

$$k_F = \left(\frac{d(2\pi)^d}{gS_d}\frac{N}{L^d}\right)^{1/d} \tag{383}$$

We can substitute ρ for N/L^d. The last thing to note is that $g = 2$ here. That's because these are spin-1/2 particles, so because each particle can take one of two internal states (spin up or spin down). Putting all this together, we get

$$\boxed{k_F = \left(\frac{d(2\pi)^d}{2S_d}\rho\right)^{1/d}} \tag{384}$$

(b) By (378), the density of states is given by

$$\rho_E\, dE = g\frac{d^dp\, d^dx}{h^d}$$

We can replace d^dx by the volume L^d, since the energy does not depend on the position:

$$\rho_E\, dE = g\frac{L^d}{h^d}\, d^dp$$

This integrand is spherically symmetric, so we can replace the integration measure d^dp with a single integration measure dp:

$$d^dp = (\text{Surface area of } d\text{-dimensional hypersphere}) \cdot p^{d-1}dp = S_d\, p^{d-1}\, dp \tag{385}$$

We can therefore write

$$\rho_E \, dE = g \frac{L^d}{h^d} S_d \, p^{d-1} \, dp \tag{386}$$

We now need to change variables from p to E, using the relation for free particles valid for this problem:

$$E = \frac{p^2}{2m}; \quad \text{so} \quad p = (2mE)^{1/2} \quad \text{and} \quad dE = \frac{p}{m} dp \tag{387}$$

Substituting in these values, we get

$$\begin{aligned}
\rho_E \, dE &= g \frac{L^d}{h^d} S_d \, p^{d-1} \, dp \\
&= g \frac{L^d}{h^d} S_d \, p^{d-2} \; p \, dp \\
&= g \frac{L^d}{h^d} S_d \, (2mE)^{(d-2)/2} \; p \left(\frac{m}{p} dE \right) \\
&= g \frac{L^d}{h^d} S_d \, (2mE)^{(d/2)-1} \; (m dE) \\
&= g \frac{L^d}{h^d} S_d \frac{(2mE)^{d/2}}{2E} \, dE \\
&= \frac{L^d}{h^d} S_d \frac{(2mE)^{d/2}}{E} \, dE \quad \text{since } g = 2 \text{ for a spin-1/2 particle}
\end{aligned}$$

Therefore, we have

$$\rho_E = \left(\frac{L^d}{h^d} S_d \right) \frac{(2mE)^{d/2}}{E} \tag{388}$$

All that remains is to write this in terms of the Fermi energy. From part (a), we know that since $g = 2$, we have (382)

$$N = 2 \left(\frac{L^d}{h^d} S_d \right) \frac{p_F^d}{d}$$

Using the fact that $E_F = \frac{p_F^2}{2m}$, we can rewrite this relation in terms of E_F:

$$N = 2 \frac{L^d}{h^d} S_d \frac{(2mE_F)^{d/2}}{d} \quad \Longrightarrow \quad \frac{L^d}{h^d} S_d = \frac{Nd}{2} \frac{1}{(2mE_F)^{d/2}} \tag{389}$$

Plugging this into (388), we get

$$\begin{aligned}
\rho_E &= \left(\frac{L^d}{h^d} S_d \right) \frac{(2mE)^{d/2}}{E} \\
&= \left(\frac{Nd}{2} \frac{1}{(2mE_F)^{d/2}} \right) \frac{(2mE)^{d/2}}{E} \\
&= N \frac{d}{2E} \left(\frac{E}{E_F} \right)^{d/2}
\end{aligned} \tag{390}$$

The problem asks for the density of states *per unit volume*, which is equal to the density of states divided by the volume L^d:

$$\begin{aligned}
D(E) = \frac{\rho_E}{L^d} &= \frac{N}{L^d} \frac{d}{2E} \left(\frac{E}{E_F} \right)^{d/2} \\
&= \rho \, \frac{d}{2E} \left(\frac{E}{E_F} \right)^{d/2} \quad \text{since } \rho = \frac{N}{L^d}
\end{aligned} \tag{391}$$

Therefore, the density of states per unit volume is

$$\boxed{D(E) = \rho\,\frac{d}{2E}\left(\frac{E}{E_F}\right)^{d/2} = \rho\,\frac{d}{2E_F}\left(\frac{E}{E_F}\right)^{d/2-1}} \tag{392}$$