Physics 725: Assignment 5

(to be submitted by Thursday, April 11, 2019)

1. The fermi function $f(\epsilon) = (e^{\beta\epsilon} + 1)^{-1}$ has some interesting properties. In particular,

$$
\begin{aligned}
f(\epsilon - \mu) &= 1 - f(\mu - \epsilon) \\
\text{and} \quad -f'(\epsilon - \mu) &= \frac{1}{k_B T} f(\epsilon - \mu) f(\mu - \epsilon) \xrightarrow{T \to 0} \delta(\epsilon - \epsilon_F).
\end{aligned}
$$

   Prove these identities, and try to give me an explanation of the physical significance of each. [*Hint:* to show that a function is a delta distribution, you need to show that it vanishes pointwise $\delta(x - x_0) = 0$ for all $x \neq x_0$ and that $\int_{-\infty}^{\infty} \delta(x - x_0) = 1$.]

2. Famously, the fermi function also admits a low-temperature expansion

$$
f(\epsilon - \mu) = \theta(\mu - \epsilon) + \frac{\pi^2}{6\beta^2}\delta'(\epsilon - \mu) + \frac{7\pi^4}{360\beta^4}\delta'''(\epsilon - \mu) + \cdots
$$

   (a) To prove this, first show that

$$
\int_{-\infty}^{\infty} g(\epsilon) f(\epsilon - \mu) = \int_{-\infty}^{\mu} g(\epsilon) + \frac{1}{\beta}\int_0^{\infty} dx\, \frac{g(\mu + x/\beta) - g(\mu - x/\beta)}{e^x + 1}
$$

   and then expand the second integral on the right-hand-side order by order in $k_B T = 1/\beta$.

   (b) The electrons in a regular material have dispersion relation $\epsilon_{\boldsymbol{k}}$ and chemical potential μ. Show that their density, expressed as a spectral integral

$$
\begin{aligned}
n = \frac{N}{V} &= \frac{2}{V}\sum_{\boldsymbol{k} \in \mathrm{BZ}} f(\epsilon_{\boldsymbol{k}} - \mu) \xrightarrow{\text{large volume}} 2\int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} f(\epsilon_{\boldsymbol{k}} - \mu) \\
&= 2\int d\epsilon\, \underbrace{\left[\int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\delta(\epsilon - \epsilon_{\boldsymbol{k}})\right]}_{\text{density of states, } D(\epsilon)} f(\epsilon - \mu) = 2\int d\epsilon\, D(\epsilon) f(\epsilon - \mu),
\end{aligned}
$$

   has a low-temperature expansion

$$
n(T) = n(T = 0) + 2\int_{\epsilon_F}^{\mu(T)} d\epsilon\, D(\epsilon) + \frac{\pi^2}{3\beta^2} D'(\mu) + O(\beta^{-4}).
$$

   Furthermore, show that the temperature dependence of the chemical potential is given by

$$
\mu \approx \epsilon_F - \frac{\pi^2 k_B^2 D'(\epsilon_F)}{6D(\epsilon_F)} T^2,
$$

   where $\mu(T = 0) = \epsilon_F$ is the fermi energy.

3. Let $D_d(\epsilon)$ be the density of states of free electrons in d spatial dimensions—i.e., $H = -\hbar^2\nabla^2/2m$ where $\boldsymbol{\nabla} = (\partial/\partial x_1, \partial/\partial x_2, \ldots, \partial/\partial x_d)$.

   (a) Find an expression for $D_d(\epsilon)$ up to an overall multiplicative constant.

   (b) Show that at temperatures much below the fermi energy, the energy per particle is

$$
\frac{E}{N} = \frac{\int d\epsilon\, D_d(\epsilon)\epsilon f(\epsilon - \mu)}{\int d\epsilon\, D_d(\epsilon) f(\epsilon - \mu)} = \frac{d}{d + 2}\epsilon_F.
$$

(c) As d gets larger, the energy per particle approaches the Fermi energy ($E/N \to \epsilon_\mathrm{F}$ as $d \to \infty$). Explain why this is so. [*Hint:* Think about the relative contributions of the "fermi surface" and the rest of the "fermi sea".]

4. On a linear chain of sites spaced by a distance a, a tight-binding model with nearest-neighbour hopping t has the dispersion relation $\epsilon_k = -2t \cos ka$. The corresponding density of states is given by

$$D_1(\epsilon) = \frac{1}{L} \sum_k \delta(\epsilon - \epsilon_k).$$

The sites are L/a in number, and the total length of the chain is L.

(a) In the thermodynamic limit ($L \to \infty$), D_1 has a closed form expression. Show that

$$D_1(\epsilon) = \frac{\theta(4t^2 - \epsilon^2)}{\pi a \sqrt{4t^2 - \epsilon^2}}.$$

(b) What is the leading order singular behaviour of D_1 as measured from the bottom and top edges of the band?

(c) Show that the corresponding density of states on a d-dimensional hypercubic lattice can be defined recursively in the form of a convolution:

$$D_d(\epsilon) = \int d\epsilon' \, D_1(\epsilon') D_{d-1}(\epsilon - \epsilon').$$

(d) Plot the density of states for $d = 1, 2, 3$ and speculate about its form in the limit $d \to \infty$. In each case, be careful to indicate the position and nature of the Van Hove singularities.

(e) The low-temperature electronic specific heat (at constant volume) is given by

$$C_V = \frac{\pi}{3} k_\mathrm{B}^2 T D_d(\epsilon_\mathrm{F}).$$

For each of $d = 1, 2, 3$, determine at which electron density C_V takes its largest and smallest values.