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PHYS 403 HW4 Model Solution

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1 Degenerate Fermions

1(a): You are given a metal which has a density of conducting electrons of $10^{29}m^{-3}$. Treating these electrons as though they were a non-interacting gas of fermions, find the $T \to 0$ values for (i) the Fermi energy, in eV; (ii) the Fermi wavelength of electrons at the Fermi surface, and (iii) the density of states at the Fermi energy.

Solution:

The particle number is given by:

$$N = V \int_0^{+\infty} dE\ g(E)\ f_F(E, \mu, T) \tag{1.1}$$

where $g(E)$ is the density of state function, and f_F is the fermion distribution function. In the limit $T \to 0$, the funciton f_F reduces to a theta function: $f_F = 0$ if $E > E_f$ and $f_F = 1$ if $E < E_f$, where E_f is the fermi energy. Therefore the integral (1.1) reduces to

$$N = V \int_0^{E_f} dEg(E) \tag{1.2}$$

in the $T \to 0$ limit. The density of state $g(E)$ in 3d is $g(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$. Thus the integral is

$$N = V\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^{E_f} dE\ E^{1/2} \tag{1.3}$$

$$= V\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{2}{3}E_f^{3/2} = V\frac{1}{3\pi^2}\left(\frac{2mE_f}{\hbar^2}\right)^{3/2} \tag{1.4}$$

$$\Rightarrow E_f = \frac{\hbar^2}{2m}\left(3\pi^2\frac{N}{V}\right)^{2/3} = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} \tag{1.5}$$

The fermi wavelength is defined via $E_f = \frac{\hbar^2 k_f^2}{2m}$, $\lambda_f = 2\pi/k_f$, therefore $k_f^2 = (3\pi^2 n)^{2/3} \Rightarrow k_f = (3\pi^2 n)^{1/3}$. Finally we evaluate the density of state at the fermi energy: $g(E_f) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_f^{1/2} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left(\frac{\hbar^2}{2m}\right)^{1/2}(3\pi^2 n)^{1/3} = \frac{3m}{(3\pi^2)^{2/3}\hbar^2}n^{1/3}$.
Substitute $n = 10^{29}$ in the above expressions, we have $E_f = 7.86$ eV, $k_f = 1.44 \times 10^{10} m^{-1} \Rightarrow \lambda_f = 2\pi/k_f = 4.375 \times 10^{-10} m$, $g(E_f) = 1.19 \times 10^{47} J^{-1}m^{-3} = 1.91 \times 10^{28}eV^{-1}m^{-3}$

Marking scheme:

1. 5 for knowing the relation (1.2)
2. 5 for getting the expression for E_f
3. 5 for getting the expression for λ_f
4. 5 for getting the expression for $g(E_f)$

1(b): A popular model for a metal (because it is so simple) is to pick a density of states:

$$g(E) = \frac{N_0}{D_0}[\theta(E + D_0) - \theta(E - D_0)] \tag{1.6}$$

Here the energy $2D_0$ is called the bandwidth of the metal, and N_0 is the number of conduction electrons per unit volume; we also assume that the $T = 0$ chemical potential is at energy $\mu = 0$.

Derive, for this system, the electronic specific heat $C_V(T)$ and the temperature dependence of the chemical potential $\mu(T)$, for low temperatures (ie., for $k_B T \ll D_0$), up to terms $\propto T^2$.

Solution:

The chemical potential is determined by

$$n = \int_{-D_o}^{+D_o} dE\, g(E) f_F(E, \mu, T) \tag{1.7}$$

To use the Sommerfeld expansion, define $h(E) := \int_{-D_o}^{E} g(\epsilon) d\epsilon$. Then the integration can be approximated by:

$$n = h(\mu) + \frac{\pi^2}{6}(kT)^2 h''(\mu) \tag{1.8}$$

The function h can be found by integrating the density of state:

$$h(E) = \int_{-D_o}^{E} \frac{N_0}{D_0}[\theta(E + D_0) - \theta(E - D_0)] = \frac{N_0}{D_0}(E + D_o),\ \forall - D_0 \le E \le D_0 \tag{1.9}$$

Therefore we have $h'' = 0$(in the region $-D_0 \le E \le D_0$), and $n = \frac{N_0}{D_0}(\mu + D_o) \Rightarrow \mu = n\frac{D_0}{N_0} - D_o = 0$.

For the energy, we use

$$h_U := \int_{-D_o}^{E} d\epsilon\, \epsilon g(\epsilon) = \frac{N_0}{2D_0}(E^2 - D_o^2),\ \ - D_0 \le E \le D_0 \tag{1.10}$$

Then energy density is given by

$$U/V = \int_0^{+\infty} dE\, Eg(E) f_F(E, \nu, T) \cong h_U(\mu) + \frac{\pi^2}{6}(kT)^2 h_U''(\mu) \tag{1.11}$$

$$= -\frac{N_0 D_o}{2} + \frac{\pi^2}{6}(kT)^2 \frac{N_0}{D_0} \tag{1.12}$$

C_V is found by taking a derivative of U:

$$C_V = dU/dT = V\left(\frac{\pi^2}{3}k^2\frac{N_0}{D_0}\right)T \tag{1.13}$$

Marking scheme:

1. 5 for knowing the Sommerfeld expansion.
2. 5 for getting μ via Sommerfeld expansion.(As long as it's a constant)
3. 5 for getting U via Sommerfeld expansion. (As long as it's quadratic in T)
4. Since $\mu = 0$ exactly in this question, you also get full points if you complete the integral for n without using Sommerfeld expansion and get the correct μ equation.

1(c): A popular model for a semiconductor has a density of states (with A_o, B_o both constants):

$$g(E) = g_o[A_o\theta(E-\Delta_0)\sqrt{E-A\Delta_o} + B_o\theta(-E-\Delta_o)\sqrt{-E-\Delta_o}] \tag{1.14}$$

We assume that at $T = 0$, all states are in the lower "valence band" are full, whereas all states in the upper "conduction band" are empty. Show that (i) if $A_o = B_o$, then $\mu(T) = 0$ for all $T > 0$, whereas if $A_o > B_o$, $\mu(T) < 0$, for $T > 0$.

Solution:

This question needs to be handled with proper care. At $T = 0$, the $E < -\Delta_o$ brance of the density of state is full, which could host infinite many electrons. For example, if one calculates the electron density N/V at $T = 0$:

$$N/V = \int_{-\infty}^{-\Delta_o} dE g_o B_0\sqrt{-E-\Delta_o} \tag{1.15}$$

it's easily seen that the integral diverges. In fact, the integral for the lower branch diverges for nonzero T as well. We can introduce a cutoff Λ to "renormalize" the integral:

$$n = \int_{-\Lambda}^{-\Delta_o} dE g_0 B_0\sqrt{-E-\Delta_o} \tag{1.16}$$

In the end of the calculation we will take the cutoff Λ to $+\infty$ but keep it finite in intermidiate steps.

Now at finite temperature we have relation

$$n = g_o A_o\int_{\Delta_o}^{+\infty}\frac{\sqrt{E-\Delta_o}}{e^{\beta(E-\mu)}+1}dE + g_o B_o\int_{-\Lambda}^{-\Delta_o}\frac{\sqrt{-E-\Delta_o}}{e^{\beta(E-\mu)}+1}dE \tag{1.17}$$

use the relation (1.16) at zero T,we have:

$$\int_{-\Lambda}^{-\Delta_o} dE g_0 B_0 \sqrt{-E-\Delta_o} = g_o A_o \int_{\Delta_o}^{+\infty} \frac{\sqrt{E-\Delta_o}}{e^{\beta(E-\mu)}+1} dE + g_o B_o \int_{-\Lambda}^{-\Delta_o} \frac{\sqrt{-E-\Delta_o}}{e^{\beta(E-\mu)}+1} dE \tag{1.18}$$

$$\Rightarrow \int_{-\Lambda}^{-\Delta_o} dE g_o B_o \left(1-\frac{1}{e^{\beta(E-\mu)}+1}\right) \sqrt{-E-\Delta_o} = g_o A_o \int_{\Delta_o}^{+\infty} \frac{\sqrt{E-\Delta_o}}{e^{\beta(E-\mu)}+1} dE \tag{1.19}$$

$$\Rightarrow \int_{-\Lambda}^{-\Delta_o} dE g_o B_o \left(\frac{\sqrt{-E-\Delta_o}}{e^{-\beta(E-\mu)}+1}\right) = g_o A_o \int_{\Delta_o}^{+\infty} \frac{\sqrt{E-\Delta_o}}{e^{\beta(E-\mu)}+1} dE \tag{1.20}$$

Notice now the LHS is convergent when we take $\Lambda \to +\infty$, because the sign of E on the expoential is now negative. Take $\Lambda \to \infty$, and define $\epsilon = -E - \Delta_o$ on the LHS and $\epsilon = E - \Delta_o$ on the RHS, we have:

$$g_o A_o \int_0^{+\infty} \frac{\sqrt{\epsilon} d\epsilon}{e^{\beta(\epsilon+\Delta_o-\mu)}+1} = g_o B_o \int_0^{+\infty} \frac{\sqrt{\epsilon} d\epsilon}{e^{\beta(\epsilon+\Delta_o+\mu)}+1} \tag{1.21}$$

when $A_o = B_o$ the equation has the obvious solution $\mu = 0$; when $A_o > B_o$, notice LHS is an increasing function of μ while the RHS is a decreasing function of μ, therefore μ must decrease from zero when A_o increases from B_o, i.e. $\mu < 0$ when $A_o > B_o$.

Marking scheme

1. 5 for knowing relation (1.2).
2. 5 for showing $\mu = 0$.
3. 5 for showing $\mu < 0$.
4. you get full marks if you are able to argue that the number of particles in the upper band equals the number of holes in the lower band.
5. 10 points off for any sort of approximate analysis, since the question is about "any $T > 0$".

2(a): For a particle in the n-th level in the well, at energy $-n\epsilon_o$, find the WKB tunneling probability $\Gamma_Q^{(n)}$ through the barrier at this energy (assume the particle has mass M), using the form given for the barrier potential $V(X)$.

Solution:

The WKB tunneling probability is

$$\Gamma = \exp\left(-\frac{2}{\hbar}\int_{x_0}^{x_1} dx\ \sqrt{2m(V(x)-E)}\right) \tag{1.22}$$

where x_0, x_1 is found by solving $V(x) = E$, here we have $V(x) = -\alpha x^2$, giving two solutions

$x_0 = -\sqrt{\frac{-E}{\alpha}}, x_1 = \sqrt{\frac{-E}{\alpha}}$, denote them as $\pm x_E$, then

$$\Gamma = \exp\left(-\frac{2}{\hbar}\int_{-x_E}^{x_E} dx\ \sqrt{2m(-\alpha x^2 - E)}\right) \tag{1.23}$$

$$= \exp\left(-\frac{2}{\hbar}\sqrt{-2mE}\int_{-x_E}^{x_E} dx\ \sqrt{1+\frac{\alpha}{E}x^2}\right) \tag{1.24}$$

$$= \exp\left(-\frac{2}{\hbar}\sqrt{-2mE}\sqrt{\frac{E}{-\alpha}}\int_{-1}^{1} dy\ \sqrt{1-y^2}\right) \tag{1.25}$$

$$= \exp\left(\sqrt{\frac{2m}{\alpha}}\frac{E}{\hbar}\pi\right) \tag{1.26}$$

where defined $y = \sqrt{\frac{-\alpha}{E}}x$ and notice the integral over y is the area of upper half of a unit circle. Now plug in $E_n = -n\epsilon$, we have

$$\Gamma_Q^{(n)} = \exp\left(-\frac{n\epsilon_o\pi}{\hbar}\sqrt{\frac{2m}{\alpha}}\right) \tag{1.27}$$

Marking scheme

1. 10 for knowing the WKB approximation (1.22).
2. 5 for getting the correct x_0, x_1.
3. 5 for completing the integral and getting the correct $\Gamma_Q^{(n)}$.

2(b): Now, let us assume that the total transition rate $\Gamma(T)$ out of the potential well is given by

$$\Gamma(T) = \sum_{n=0}^{N} \Gamma_Q^{(n)} \exp\left[-\beta\epsilon_n\right] \tag{1.28}$$

Here $\beta = 1/k_B T$, and we sum over all the levels from the lowest energy state at energy $E_N = -N\epsilon_o$, up to the highest energy state at top of the barrier, at energy $E_o = 0$.

Show that at low T the transition is dominated by the transitions from the lowest state at energy $E_N = -N\epsilon_o$ whereas at high T, it is dominated by transitions from the state at the top of the barrier, at energy $E_o = 0$. Show also that there is an intermediate 'crossover' temperature Tc at which the transition rate from each of the levels is roughly the same; and find T_c as a function of the parameters α and k_B.

Solution

Write $\Gamma_Q^{(n)} = e^{-n\Delta}$ with $\Delta = \frac{\epsilon_o \pi}{\hbar}\sqrt{\frac{2m}{\alpha}}$. The total probability is

$$\Gamma(T) = \sum_{n=0}^{N} \Gamma_Q^{(n)} e^{\beta n \epsilon_o} = \sum_{n=0}^{N} e^{n(-\Delta + \beta\epsilon_o)} \tag{1.29}$$

At low T, β is large, the overall coefficient $-\Delta + \beta\epsilon_o$ is positive, therefore the $n = N$ term is largest. At high T, $-\Delta + \beta\epsilon_o \simeq -\Delta$ is negative, therefore the term with $n = 0$ is largest. When $-\Delta + \beta\epsilon_o = 0$, all terms contribute equally. The solution is

$$\beta = \frac{\Delta}{\epsilon_o} = \frac{\pi}{\hbar}\sqrt{\frac{2m}{\alpha}} \Rightarrow T_c = \frac{\hbar}{\pi k_B}\sqrt{\frac{\alpha}{2m}} \tag{1.30}$$

Marking scheme

1. 10 for arriving at the correct $\Gamma(T)$ expression.
2. 10 for showing the correct large and small T analysis.
3. 10 for getting the crossover value T_c.