Solid State Theory
Exercise 6

Exercise 6.1 Specific Heat of a Metal, a Semiconductor, and Graphene

a) Calculate the specific heat of a metal for small temperatures $k_B T \ll \mu$ by using the Bohr-Sommerfeld expansion

$$\int_{-\infty}^{\infty} d\epsilon \, \frac{H(\epsilon)}{e^{(\epsilon-\mu)/k_B T}+1} = \int_{-\infty}^{\mu} d\epsilon \, H(\epsilon) + \sum_{n=1}^{\infty} a_n \left(k_B T\right)^{2n} \left.\frac{d^{2n-1}H(\epsilon)}{d\epsilon^{2n-1}}\right|_{\epsilon=\mu} \tag{1}$$

where $a_1 = \pi^2/6$, $a_2 = 7\pi^4/360, \ldots$.

Hint:
We use the Jellium model to describe the metal, i.e. we assume free electrons with the dispersion relation

$$\epsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m} \tag{2}$$

which occupy all states which satisfy $\epsilon_{\vec{k}} < \epsilon_F$ at $T = 0$. Compute the density of states and calculate the particle density $n(\mu, T)$ and the energy density $u(\mu, T)$ up to second order in T. In order to express u in terms of n and T, determine the chemical potential μ by fixing the particle density.

b) Calculate the specific heat of a semiconductor under the assumption $k_B T \ll E_g$, where E_g is the band gap. Show that it is given by an ideal gas-like part $(3/2)n(T)k_B$ plus a correction, where $n(T)$ is the number of excitations. Is this correction small or large?

Hint:
First, approximate the dispersion of both the conduction and the valence band parabolically, with the two effective masses m_v and m_c. Then, calculate the chemical potential μ from the condition, that the number of electrons in the conduction band $(n_e(T))$ must be equal to the number of holes in the valence band $(n_h(T))$.

c) Calculate the specific heat of graphene close to the Dirac point at half filling.

Hint:
Near the Dirac point the dispersion is linear and given by

$$E = \pm \hbar v_F |\vec{k}|, \tag{3}$$

such that the origin is at the Fermi energy ($\epsilon_F = 0$). To find the temperature dependence of the chemical potential, use a two-band approach (semiconductor with gap going to zero). Calculate the density of states and the number of mobile electrons in the conduction bands. For the internal energy, consider $u(T) - u_0$.

Exercise 6.2 Spin Susceptibility of a Metal, a Semiconductor, and Graphene

a) Calculate the Pauli spin susceptibility of a metal due to its conduction electrons, neglecting any orbital effects.

Hint:
How does an external magnetic field H coupling to the electron spins $s = \pm 1$ change their energy and how does this affect the particle density n? Define the magnetization through the different particle densities for up and down spins ($n_s(H)$) to find the susceptibility χ_{Pauli}.

b) Calculate the spin susceptibility of a semiconductor and compare it to an ideal paramagnetic gas.

Hint:
Use the same idea as for the metal but mind the gap. Consider electrons and holes separately and argue how their contributions are related. We again work under the assumption that $k_B T \ll E_g$.

c) Calculate the spin susceptibility of graphene.

Hint:
Use a two-band approach and again the same idea as for the metal.

Exercise 6.3 Easter Special:
Density of States from the Tight-Binding Model

Calculate the density of states for the 1d, 2d and 3d tight-binding model on a square lattice. The band structure (we set $a \equiv 1$) is given by

$$\epsilon(\vec{k}) = -2t \sum_i \cos k_i, \tag{4}$$

where i runs over all dimensions.

Hint:
For 1d you can find the solution analytically, while for 2d and 3d you may use numerics. Approximate the δ-function by a Cauchy distribution of width δ and use N lattice points. Compute the sum with Matlab for different values of δ and N. What relation (and values) of N and $1/\delta$ do you need for a good result?

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