

September 9, 2021

HOMEWORK 3
OPTI 507
(due September 16, 2021)

Problem 1:

In class we discussed a convenient and general expression for the density of states of a two-fold (for spin) degenerate band with band energies $\varepsilon_{\nu,\mathbf{k}}$,

$$g_{\nu}(\varepsilon) = 2 \frac{1}{V} \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\nu,\mathbf{k}}) \quad (1)$$

where, in the large volume limit, $\frac{1}{V} \sum_{\mathbf{k}}$ is to be interpreted as an appropriate integral (as discussed in class). Using this form for the density of states, find an analytical expression for the density of states of a 2-fold degenerate parabolic band, $\varepsilon_{\nu,\mathbf{k}} = \varepsilon_{\nu,0} + \frac{\hbar^2 k^2}{2m_{\nu}}$, in a 3-dimensional crystal.

(10 points)

Problem 2:

Show that the wavefunctions for the 3-dimensional tight binding model

$$\varphi_{\nu\vec{k}}(\vec{r}) = \mathcal{N} \sum_n e^{i\vec{k}\cdot\vec{R}_n} \phi_{\nu}(\vec{r} - \vec{R}_n) \quad (2)$$

where \mathcal{N} is an appropriate normalization factor and n stands for (n_1, n_2, n_3) , satisfy Bloch's theorem.

(10 points)

Problem 3:

In order to understand the difference between a semiconductor and a metal, one needs to understand that in a semiconductor the chemical potential is between the valence and conduction band. This problem shows the exact position of the chemical potential in a semiconductor.

Consider a semiconductor with a 6-fold degenerate parabolic conduction band and a 6-fold degenerate parabolic valence band, separated by the energy gap E_G (most semiconductors have 2-fold degenerate bands, the 6-fold degeneracy is only used in this problem). Determine the chemical potential μ as function of temperature T , and show that in the zero-temperature limit μ is exactly half way between the valence and conduction band. You may assume that the chemical potential is sufficiently far from both the conduction and the valence band so that the Fermi functions for the appropriate particle species (not necessarily electrons!) can be approximated by Maxwell-Boltzmann distributions. INSTRUCTIONS: Do not follow the book when solving this problem. In particular, do NOT use the concept of density of states (DOS). Integrate all k-integrals directly; all of them can be reduced to the form

$$\int_0^{\infty} dx x^2 e^{-a^2 x^2} = \frac{\sqrt{\pi}}{4a^3} \quad (3)$$

(10 points)