

Physics 880.06: Problem Set 7

Due Friday, November 15, 2002

Note: each problem is worth 10 pts.

1. *One-dimensional tight-binding model with two atoms per primitive cell.* Consider a one-dimensional lattice of atoms of two types, A and B, which alternate. Assume that the spacing between atoms is a . We choose our origin so that the zeroth primitive cell extends between $x = -a$ and $x = +a$; the A and B atoms in that cell are located at $x = -a/2$ and $x = +a/2$. Let each type of atom have one atomic orbital, which we denote ϕ_A and ϕ_B . Thus, we write the orbital for atoms of type A and type B in the n^{th} primitive cell as $\phi_A(\mathbf{r} + \hat{x}/2 - \mathbf{R}_n)$ and $\phi_B(\mathbf{r} - a\hat{x}/2 - \mathbf{R}_n)$, where $\mathbf{R}_n = 2na\hat{x}$. You may think of the functions $\phi_A(\mathbf{r})$ and $\phi_B(\mathbf{r})$ as spherically symmetric and centered at $\mathbf{r} = 0$. Note: this notation is slightly different from that used in class.

Now assume that the matrix elements of the Hamiltonian with respect to these atomic orbitals vanish except for the diagonal elements and between nearest neighbors. We assume that these elements have the following values:

$$\begin{aligned}\int \phi_A^*(\mathbf{r} + a\hat{x}/2)H\phi_A(\mathbf{r} + a\hat{x}/2)d^3x &= \epsilon_A \\ \int \phi_B^*(\mathbf{r} - a\hat{x}/2)H\phi_B(\mathbf{r} - a\hat{x}/2)d^3x &= \epsilon_B \\ \int \phi_A^*(\mathbf{r} + a\hat{x}/2)H\phi_B(\mathbf{r} - a\hat{x}/2)d^3x &= -t_1 \\ \int \phi_A^*(\mathbf{r} + a\hat{x}/2)H\phi_B(\mathbf{r} + 3a\hat{x}/2)d^3x &= -t_2,\end{aligned}$$

where we assume that both t_1 and t_2 are real and positive, but not necessarily equal.

You may assume that the orbitals centered on different atomic sites are orthonormal, and that the Hamiltonian is periodic, as discussed in class.

- (a). What is the first Brillouin zone of this 1D lattice?
- (b). The band energies at wave number k are the solutions of a 2×2 determinantal equation. Find that equation.
- (c). Solve to find the band energies $E(k)$. There will be two bands. Evaluate these band energies explicitly for $k = 0$ for k at the edges of the Brillouin zone. Show that the energies at the zone edge become degenerate when $t_1 = t_2$ and $\epsilon_A = \epsilon_B$.
2. Ashcroft and Mermin, Chapter 22, Problem 1 (a) and (b) only.
3. In class we calculated the normal modes of a one dimensional lattice consisting of two alternating types of masses, M_1 and M_2 , connected by springs of spring constant K . Generalize this calculation to find the normal modes of a one-dimensional lattice consisting of two alternating masses M_1 and M_2 , connected by two alternating types of springs, of spring constants K_1 and K_2 . Assume that the equilibrium separation of adjacent masses is a .
- (a). Find the dispersion relations for the acoustic and optical phonon branches.
- (b). Find the vibrational frequencies at (i) $k = \pm\pi/(2a)$ and (ii) $k = 0$. Show that, in case (i), the frequencies of the two modes at $k = \pi/(2a)$ become equal when $K_1 = K_2$ and $M_1 = M_2$.