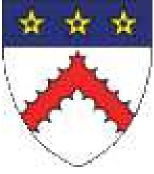

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Keble College - Hillary 2010

B2: Condensed Matter Physics and Photonics

Tutorial 6 - Tight Binding Model and Semiconductors

Please leave your work in my Keble pigeon hole by 5pm on Wednesday of 3rd week.
Suggested reading: Hook & Hall 4, 5; Kittel 8; Ashcroft/Mermin 28.

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1 The Tight Binding Model

In the last tutorial we saw how band theory emerges from a nearly free electron model with a small crystal potential. The other extreme is the *tight binding model*, where we begin by assuming electrons are tightly bound to their 'parent atoms', and then examine the effects of introducing neighbours. First we consider the properties of one electron in the presence of two atoms.

1. Consider a single electron interacting with two protons at the fixed positions $\mathbf{R}_n$ and $\mathbf{R}_m$. The Hamiltonian for such an electron is

$$H = \frac{-\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}-\mathbf{R}_n|} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}-\mathbf{R}_m|}.$$

Without doing any calculations explain what you expect for the eigenfunctions and eigenvalues in the limits (a) $|\mathbf{R}_n - \mathbf{R}_m| \gg a_B$, and (b) $|\mathbf{R}_n - \mathbf{R}_m| \ll a_B$, where a_B is the Bohr radius.

We will now consider an intermediate regime. Let $|n\rangle$ denote the state in which the electron is bound to atom n with the isolated atom eigenstate $\phi(\mathbf{r} - \mathbf{R}_n)$ (eigenvalue E_0), and similarly for $|m\rangle$. Show that if we use the trial orthogonal eigenstates:

$$|E_\pm\rangle = \frac{1}{\sqrt{A_\pm}}(|n\rangle \pm |m\rangle), \tag{1}$$

Our energies are:

$$E_\pm \approx \frac{1}{A_\pm}\left(2E_0 - \langle n|\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}-\mathbf{R}_m|}|n\rangle - \langle m|\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}-\mathbf{R}_n|}|m\rangle \pm \Big\{\langle n|H|m\rangle + \langle m|H|n\rangle\Big\}\right). \tag{2}$$

Where $A_\pm$ is a normalization constant. Why is the term in braces is called a *hopping integral*?

2. We now extend these ideas to the many body case, limiting our attention to a particularly simple example of the tight binding model. Considering a one dimensional monoatomic chain and a single atomic orbital, the Hamiltonian for a single electron is given by:

$$H = \sum_n^N \big(\varepsilon|n\rangle\langle n| \quad - \quad t|n+1\rangle\langle n| \quad - \quad t|n-1\rangle\langle n|\big). \tag{3}$$

Here, N is the number of atoms in the system, ε is the energy of the atomic orbital and t is a hopping integral, with the simplifying assumption $\langle n|m\rangle = \delta_{n,m}$.

Define $|k\rangle$ states by

$$|n\rangle = \frac{1}{\sqrt{N}}\sum_k e^{-ikna}|k\rangle \quad , \quad \langle n| = \frac{1}{\sqrt{N}}\sum_k e^{ikna}\langle k| \tag{4}$$

with a as the lattice parameter. By substituting Eqn. 4 into Eqn. 3, show that the Hamiltonian diagonalises to

$$H = \sum_k \big(\varepsilon - 2t\cos(ka)\big) \mid k\rangle\langle k \mid .$$

Sketch the dispersion relation and illustrate the filling in the monovalent case (assuming the electrons do not interact with each other).

2 Electrons, Holes and Semiconductors

3. Please attempt question C5 from Prof. Robin Nicholas's problem set.

4. Please attempt question C6 from Prof. Robin Nicholas's problem set.

5. Explain the terms *group velocity* and *effective mass* as applied to an electron in a crystal. How can a negative effective mass be reconciled with the fact that the mass of a free electron is positive? [5]

   Consider an electron in a one dimensional energy band $E(k_x)$, where k_x is the wavevector along the x-direction. An electric field F is applied along the x-direction. Show that the equation describing the motion of the electron along the x-direction is

   $$\hbar \frac{dk_x}{dt} = -eF \tag{5}$$

   Derive an expression for the effective mass in terms of the band structure $E(k_x)$. [8]

   An electron with wavevector $\mathbf{k} = (k_x, 0, 0)$ has energy

   $$E(k_x) = A\big[1 - \cos(k_x a) + \tfrac{1}{8}\cos(2k_x a)\big]$$

   where a is the lattice period and $A > 0$. Obtain expressions for the electron group velocity and effective mass along the x-direction. Sketch the variation of these two quantities as k_x varies from 0 to $\frac{\pi}{a}$. Estimate the value of k_x at which the effective mass becomes infinite. [9]

   By considering equation (5), or otherwise, describe the motion of an electron in this energy band under the influence of an external electric field along the x-direction. (Neglect any scattering effects.) [3]

   [1998 A4 question 5 (old course)]

6. Explain the principle of doping a semiconductor with impurities to produce an excess of electrons or holes. Give an example of a suitable material with which to dope silicon to produce an excess of electrons. [7]

   Give expressions for the density of free electrons (n) and holes (p) in a semiconductor in terms of the density of states in the conduction and valence bands and the Fermi-Dirac distribution function. [4]

   Using the free-electron form of the density of states and approximating the Fermi-Dirac distribution function in each case by an exponential, derive an expression for the hole and electron densities as a function of temperature and Fermi energy in a semiconductor with a band gap E_g and electron and hole effective masses of m_e^* and m_h^*. Show that the results give a product np which is independent of the Fermi energy E_F. [9]

   A material with $E_g = 1\ eV$ and $m_e^* = m_h^* = 0.1\, m_e$ is doped with $1 \times 10^{23} m^{-3}$ shallow donor impurities. Calculate the density of holes present at room temperature. [5]

   $$\left[\quad \int_0^\infty dx\, x^{1/2}\, e^{-x} = \frac{\sqrt{\pi}}{2} \quad \right]$$

   [1996 A4 question 5 (old course)]

7. Explain what the terms *direct gap* and *indirect gap* mean when used to describe semiconductors. [5]

   Show that the number of electrons per unit volume in the conduction band of an intrinsic gap semiconductor at a temperature T is given by

$$n = AT^{3/2}\exp\left(\frac{-E_g}{2k_BT}\right)$$

   where E_g is the energy gap and A is a constant which need not be evaluated. [10]

   The Hall coefficient R_H for a sample of undoped silicon is measured to be 625 m^3C^{-1} at $300K$ and 0.016 m^3C^{-1} at $500K$. Assuming only one type of carrier contributes to R_H deduce a value for E_g from these data. [6]

   The optical absorption of silicon as a function of photon energy exhibits large increases at 1.2 eV and 3.3 eV. Comment on your value for E_g in relation to these optical data. [4]

[2000 A4 question 4 (old course)]