PHY 491 - 2013

Atomic, Molecular, and Condensed Matter Physics

Problem Set 11

1. Consider a one-dimensional lattice with lattice constant a. Make a plot of the energy $E_{m\mathbf{k}}$ in the reduced-zone picture (projection on the first Brillouin zone). Disregard the periodic potential-induced corrections. Plot energy of the bands in the units of $(\pi\hbar/a)^2/2m_e$. Consider the range where the energy in these units is ≤ 9. What will be the major change of the picture if there is a weak periodic potential? (5 pt)

2. Show that, if the extra potential in the tight-binding method has inversion symmetry, $\Delta U(\mathbf{r}) = \Delta U(-\mathbf{r})$, then $\gamma(\mathbf{R}) = \int d\mathbf{r}\psi_m^*(\mathbf{r})\Delta U(\mathbf{r})\psi_m(\mathbf{r}-\mathbf{R}) = \gamma(-\mathbf{R})$, where $\mathbf{R}$ is a lattice vector and $\psi_m(\mathbf{r})$ is an s-type atomic wave function. (3 pt)

3. Calculate and plot the dispersion law in the tight-binding method for s-states in a two-dimensional square lattice with lattice constant a. Use the nearest-neighbor approximation. (4 pt)

4. Consider Wannier functions $\psi_m(\mathbf{r}-\mathbf{R}) = C\sum_{\mathbf{k}}\psi_{m\,\mathbf{k}}(\mathbf{r})\exp(-i\mathbf{k}\mathbf{R})$ where $\mathbf{R}$ is a lattice vector, the sum runs over the values of $\mathbf{k}$ in the first Brillouin zone, and $\psi_{m\,\mathbf{k}}(\mathbf{r})$ is the Bloch wave function of the mth band. The wave vectors $\mathbf{k}$ are such that $\psi_{m\,\mathbf{k}}(\mathbf{r})$ satisfies the Born-von Karman periodic boundary conditions. Show that $\int d\mathbf{r}\,\psi_m^*(\mathbf{r}-\mathbf{R})\psi_m(\mathbf{r}-\mathbf{R}') \propto \delta_{\mathbf{R},\mathbf{R}'}$. Find the normalization constant C in terms of functions $\psi_{m\,\mathbf{k}}(\mathbf{r})$. (7 pt)

5. The Hamiltonian in the tight-binding method for the mth band can be written in a compact way in terms of Wannier wave functions $\psi_m(\mathbf{r}-\mathbf{R})$ if one introduces an operator $|m;\mathbf{R}\rangle\langle m;\mathbf{R}'|$ such that $|m;\mathbf{R}\rangle\langle m;\mathbf{R}'|\psi_m(\mathbf{r}-\mathbf{R}_1) = \delta_{\mathbf{R}',\mathbf{R}_1}\psi_m(\mathbf{r}-\mathbf{R})$. One can then write the Hamiltonian in the nearest-neighbor approximation for a simple cubic lattice as

$$H = E_m\sum_{\mathbf{R}}|m;\mathbf{R}\rangle\langle m;\mathbf{R}| + t\sum_{\text{n.n.}}|m;\mathbf{R}\rangle\langle m;\mathbf{R}'| \qquad (1)$$

where the second sum runs over the nearest neighbors. Find the energy $E_{m\,\mathbf{k}}$ of an electron with momentum $\mathbf{k}$ for Hamiltonian (1). Compare with the result obtained in class and given in the textbook as applied to the nearest neighbor approximation and establish the relation between the parameters. (6 pt)

You are supposed to get 20 points. The solution is due on November 27.