Phys 771
Condensed Matter Physics
Problem Set # 6

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1. Consider a periodic potential $U(\vec{r}) = \sum_{\vec{K}} U_{\vec{K}} e^{i\vec{K}.\vec{r}}$, with a plane wave solution $< \mathbf{r}|\mathbf{k} >= \frac{1}{\sqrt{V}} e^{i\vec{k}.\vec{r}}$, show that the matrix elements of the potential $< \mathbf{k}'|U|\mathbf{k} >= U_{\mathbf{k}'-\mathbf{k}}$, i.e the only non-vanishing Fourier components of $U(\vec{r})$ are those that link different states via reciprocal lattice vectors. Find $< \mathbf{k}+\mathbf{K}|U|\mathbf{k} >$ and $< \mathbf{k}|U|\mathbf{k}+\mathbf{K} >$ and show that $U_{-\mathbf{K}} = U^*_{\mathbf{K}}$

2. Consider the 1D periodic potential $U(x) = 2\ V_o\ cos^2(\frac{\pi x}{a})$, where V_o is real constant. Use perturbation theory to find the first and second order corrections to energy and estimate the energy gap at $k = \pi/a$

3. Marder 8.1 (modified): Consider a square lattice in two dimensions with the potential

   $U(x, y) = -4U_0\ cos(\frac{2\pi x}{a})\ cos\frac{2\pi y}{a}$

   Determine the non-vanishing Fourier components of $U(x, y)$. Use the central equation to estimate the energy gap at the Brillouin zone's corner point, $(\pi/a, \pi/a)$. Simply solving a 2x2 determinantal problem is sufficient.

4. Use the tight-binding model to calculate the band structure of an ABABAB... chain (a 1D diatomic lattice with alternating atoms A and B as shown in Figure 1), assuming that the distance between any two neighboring atoms is a, and the on-site energies of A and B are ε_A and ε_B, respectively. The resulting dispersion relation should have two bands: the bottom band may be called the valence band, while the higher band can be called the conduction band. Find the bandwidth at $k = 0$ and the energy gap at $k = \pm\ \pi/2a$. Use computer to plot the two bands in the first BZ; $[-\pi/2a, \pi/2a]$. Make the plot for the two cases $\varepsilon_A \neq \varepsilon_B$ and $\varepsilon_A = \varepsilon_B$. Which case generates a band gap?

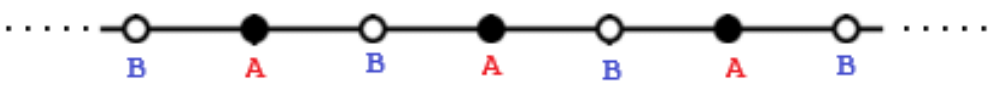

Figure 1:

5. Use the tight-binding model to calculate the band structure of a diatomic square lattice (with alternating atoms A and B, as shown in Figure 2), assuming that each unit cell contains two atoms A and B and the distance between any two neighboring atoms is a, and the on-site energies of A and B are ε_A and ε_B, respectively. The resulting dispersion relation should have two bands: the bottom band may be called the valence band, while the higher band can be called the conduction band. Use computer to plot the two bands in the first BZ; $k_x, k_y \in [-\pi/a, \pi/a]$. Make the plot for the two cases $\varepsilon_A \neq \varepsilon_B$ and $\varepsilon_A = \varepsilon_B$. Which case generates a band gap? Find the bandwidth of each band

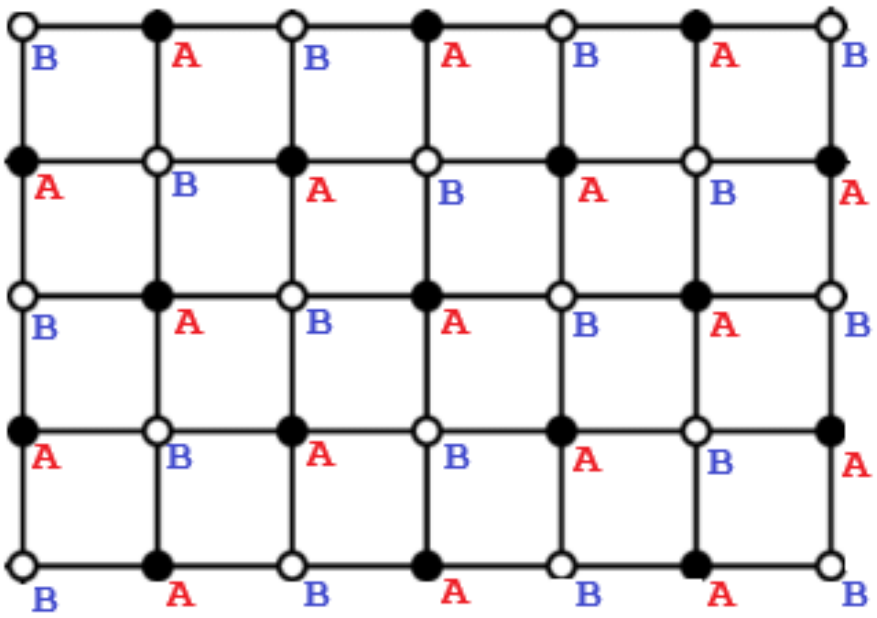

Figure 2:

6. Calculate the tight-binding density of states for the 1D diatomic chain discussed in problem 4. Use computer to plot the two density of states of the two bands in the first BZ; $[-\pi/2a, \pi/2a]$. Make the plot for the two cases $\varepsilon_A \neq \varepsilon_B$ and $\varepsilon_A = \varepsilon_B$