

Problem Set 3

due Wednesday Feb. 14, at beginning of class

Name

Student Number

(I am using **bold-face print** not arrows to indicate vectors here.)

1) Prove that if the volume of a primitive cell of a Bravais lattice is v , then the volume of a primitive cell of the corresponding reciprocal lattice is necessarily $(2\pi)^3/v$. To do this use:

a) the formula relating primitive vectors of the reciprocal and direct lattice in the Jan. 8 lecture notes

b) The formula for the volume of a parallelepiped: with sides $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$:
 $v = |(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3|$.

c) The triple product identity: $(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{b} \cdot \mathbf{c})\mathbf{a}$.

2) Consider electrons in a one dimensional crystal with periodic potential $U(x) = \epsilon_0 \cos^3(2\pi x/a)$, in the limit of small ϵ_0 .

a) Calculate all non-zero Fourier modes of the potential

$U_K = (1/a) \int_0^a dx e^{-iKx} U(x)$ with K in the reciprocal lattice.

b) In the limit $U(x) = 0$, write a formula for all energy bands in the first Brillouin zone.

c) Find the 5 lowest energy values of $[k, \epsilon(k)]$ in the first Brillouin zone where 2 energy levels become equal.

d) Write a formula for the splitting of each of these pairs of degenerate levels, in terms of the parameter ϵ_0 defined above.

e) Draw a graph of the 4 lowest energy bands, with these splittings included accurately.

3) Consider the two lowest energy bands of a one dimensional metal near the edge of the first Brillouin zone, $k = \pi/a - \delta k$ for $0 < \delta k \ll \pi/a$. For small $U(x)$, the main contribution to their energies there comes from the Fourier modes U_K with $K = 2\pi/a$.

a) Keeping only the Fourier modes $U_{\pm K}$ in the Fourier transformed Schroedinger equation derived in the Jan. 22 lecture notes, write a formula for the 2 energy levels ϵ_{\pm} in this region of k .

- b) By Taylor expanding this expression in powers of $\delta\mathbf{k}$, show that the derivatives of $\epsilon_{\pm}(\mathbf{k})$ both vanish at $k=\pi/a$, consistent with the figure in the Jan. 24 lecture notes.
- c) Now generalize this to a 3 dimensional metal which has 2 degenerate energy bands for $U=0$ at a point in the first Brillouin zone \mathbf{k}_0 , due to the fact that $(\mathbf{k}_0)^2=(\mathbf{k}_0-\mathbf{K})^2$ for some reciprocal lattice vector, \mathbf{K} . Consider values of \mathbf{k} close to \mathbf{k}_0 : $\mathbf{k}=\mathbf{k}_0+\delta\mathbf{k}$. Calculate the energy difference $\epsilon_+(\mathbf{k})-\epsilon_-(\mathbf{k})$ in this region of \mathbf{k} -space and show that this difference is generally quadratic in $\delta\mathbf{k}$, not linear.

- 4) In this problem, you will calculate two energy levels of a NaCl-like crystal using the tight-binding approximation. This crystal structure is illustrated in the Jan 5 lecture notes. It is face-centred cubic with a 2-atom basis (1 Na and 1 Cl). Label

the sites with Na atoms, \mathbf{R} (which includes the origin) and the sites with Cl atoms \mathbf{R}' . Write the Na wave-function for an atom at site \mathbf{R} as $\psi_N(\mathbf{r}-\mathbf{R})$ and write the Cl wave-function for an atom at site \mathbf{R}' as $\psi_C(\mathbf{r}-\mathbf{R}')$. Write an approximate set of wave-functions in the form:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \alpha_{\mathbf{k}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \psi_N(\mathbf{r}-\mathbf{R}) + \beta_{\mathbf{k}} \sum_{\mathbf{R}'} e^{i\mathbf{k}\cdot\mathbf{R}'} \psi_C(\mathbf{r}-\mathbf{R}')$$

Here \mathbf{k} lies in the first Brillouin zone. $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ are parameters determined to give approximate eigenfunctions. As usual, in the tight-binding approximation, we assume that the single atom wave-functions drop off rapidly on the scale of the separation of the nearest neighbour atoms (1 Na, 1 Cl), which we label a . We write two equations, which would be exact if $\psi_{\mathbf{k}}(\mathbf{r})$ was an exact eigenfunction,

$$\int d^3r \psi_N(\mathbf{r})^* H \psi_{\mathbf{k}}(\mathbf{r}) = \epsilon(\mathbf{k}) \int d^3r \psi_N(\mathbf{r})^* \psi_{\mathbf{k}}(\mathbf{r}) \quad (1)$$

$$\int d^3r \psi_C(\mathbf{r}-\mathbf{R}_0')^* H \psi_{\mathbf{k}}(\mathbf{r}) = \epsilon(\mathbf{k}) \int d^3r \psi_C(\mathbf{r}-\mathbf{R}_0')^* \psi_{\mathbf{k}}(\mathbf{r}) \quad (2)$$

Here $\mathbf{R}_0' = a(1,0,0)$ labels the location of one of the Cl atoms closest to the origin. On the right hand side of these equations we make the approximation of only keeping 1 term, $\alpha_{\mathbf{k}} \psi_N(\mathbf{r})$ in Eq. (1) and $\beta_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{R}_0') \psi_C(\mathbf{r}-\mathbf{R}_0')$ in Eq. (2).

On the left hand side of Eq. (1) we write the Hamiltonian as $H = H_{at,N} + \Delta U(\mathbf{r})$ where $H_{at,N}$ is the Hamiltonian for a single N atom at the origin (kinetic energy plus single atom potential energy). Then

$$\int d^3r \psi_N(\mathbf{r})^* H_{at,N} \psi_{\mathbf{k}}(\mathbf{r}) = E_{at,N} \int d^3r \psi_N(\mathbf{r})^* \psi_{\mathbf{k}}(\mathbf{r})$$

where $E_{at,N}$ is the single Na atom energy eigenvalue. Again we approximate the integral on the right hand side as $\alpha_{\mathbf{k}}$, only keeping the largest term. The remaining terms on the left hand side of Eq. (1) contain factors

$\int d^3r \psi_N(\mathbf{r})^* \Delta U(\mathbf{r}) \psi_N(\mathbf{r}-\mathbf{R})$ and $\int d^3r \psi_N(\mathbf{r})^* \Delta U(\mathbf{r}) \psi_C(\mathbf{r}-\mathbf{R}')$. These will drop off exponentially with increasing R and R' . We only keep the term $R=0$ in the first factor and the 6 shortest R' vectors in the second factor. We label these:

$\int d^3r \psi_N(\mathbf{r})^* \Delta U(\mathbf{r}) \psi_N(\mathbf{r}) = -\gamma_{0,N}$ and $\int d^3r \psi_N(\mathbf{r})^* \Delta U(\mathbf{r}) \psi_C(\mathbf{r}-\mathbf{R}') = -\gamma_1$, assumed to be equal for all 6 shortest R' vectors. (This would follow if the corresponding wave-functions were spherically symmetric.)

On the left hand side of Eq. (2) we write $H=H_{at,C}+\Delta U'(\mathbf{r})$ where $H_{at,c}$ is the Hamiltonian for a single Cl atom at position \mathbf{R}_0' . Then

$$\int d^3r \psi_C(\mathbf{r}-\mathbf{R}_0')^* H_{at,C} \psi_k(\mathbf{r}) = E_{at,C} \int d^3r \psi_C(\mathbf{r}-\mathbf{R}_0')^* \psi_k(\mathbf{r})$$

where $E_{at,C}$ is the single Cl atom energy eigenvalue. Again we approximate the integral on the right hand side as $\beta_k \exp(i\mathbf{k} \cdot \mathbf{R}_0')$, only keeping the largest term. The other terms contain factors

$\int d^3r \psi_C(\mathbf{r}-\mathbf{R}_0')^* \Delta U'(\mathbf{r}) \psi_C(\mathbf{r}-\mathbf{R}_0')$ and $\int d^3r \psi_C(\mathbf{r}-\mathbf{R}_0')^* \Delta U'(\mathbf{r}) \psi_N(\mathbf{r}-\mathbf{R})$. We only keep the $\mathbf{R}'=\mathbf{R}_0'$ term in the first factor and only the 6 \mathbf{R} vectors closest to \mathbf{R}_0' in the second factor. We label these

$\int d^3r \psi_C(\mathbf{r}-\mathbf{R}_0')^* \Delta U'(\mathbf{r}) \psi_C(\mathbf{r}-\mathbf{R}_0') = -\gamma_{0,C}$ and $\int d^3r \psi_C(\mathbf{r}-\mathbf{R}_0')^* \Delta U'(\mathbf{r}) \psi_N(\mathbf{r}-\mathbf{R}) = -\gamma_1^*$ for all 6 \mathbf{R} vectors closest to \mathbf{R}_0' . [Note that γ_1^* is the complex conjugate of the overlap integral occurring in Eq. (1).]

a) Use the above results to write a 2x2 matrix eigenvalue equation of the form

$$M \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \epsilon \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \text{ for each value of } \mathbf{k}. \text{ for a Hermitean, } \mathbf{k}\text{-dependent matrix } M.$$

b) Solve this eigenvalue equation to determine 2 energy bands, $\epsilon_{\pm}(\mathbf{k})$.