

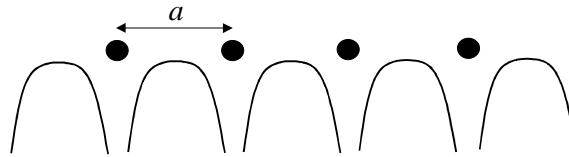
ABACUS Exercise: Bandstructure – Kronig-Penney Model and Tight-Binding Exercise

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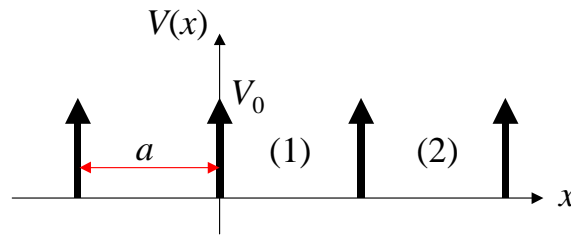
(ASU/Purdue)

Objective: The objective of this exercise is to start with the simple Kronig-Penney model and understand formations of bands and gaps in the dispersion relation that describes the motion of carriers in 1D periodic potentials. The second exercise examines the behavior of the bands at the Brillouin zone boundaries. Finally, a simplified tight-binding approach for 1D lattice has to be derived as part of the third exercise..

1. Electrons in a lattice see a periodic potential due to the presence of the atoms, which is of the form shown below:



This periodic potential will open gaps in the dispersion relation, i.e. it will impose limits on the allowed particle energies. To simplify the problem, one can assume that the width of the potential energy term goes to zero, i.e. the periodic potential can be represented as an infinite series of δ -function potentials:



- (a) Using Bloch theorem for the general form of the solution of the 1D TISE (time-independent Schrödinger equation) in the presence of periodic potential, show that the relationship between the crystal momentum and particle energy is obtained by solving the following implicit equation

$$\cos(ka) = P \frac{\sin(k_0 a)}{k_0 a} + \cos(k_0 a) , \quad (1.1)$$

where k is the crystal momentum and $E = \hbar^2 k_0^2 / 2m$. The quantity $P = 2mV_0 / \hbar^2$ in (1.1) may be regarded as the "scattering power" of a single potential spike.

- (b) Plot the dispersion relation for a particle in a periodic potential for the case when $P=2.5$.
2. In the free-electron approximation, the total energy of the electrons is assumed to be always large compared to the periodic potential energy. Writing the 1D time-independent Schrödinger wave equation in the form

$$\frac{d^2\psi}{dx^2} + [k_0^2 + \gamma f(x)]\psi(x) = 0, \quad (2.1)$$

where $E = \hbar^2 k_0^2 / 2m$ and $\gamma f(x) = 2mV(x)/\hbar^2$, it is rather straightforward to show that in the limit $\gamma \rightarrow 0$ and away from the band edge points ($\pm n\pi/a$), one can approximate the wavefunction $\psi(x)$ with

$$\psi(x) = e^{ikx} u_k(x) = e^{ikx} \sum_n b_n e^{-i2\pi nx/a} \approx b_0 e^{ikx} + \gamma e^{ikx} \sum_{n \neq 0} b_n e^{-i2\pi nx/a}. \quad (2.2)$$

- (a) Show that the result given in (2.2) is a valid approximation for $\psi(x)$ in the limit $\gamma \rightarrow 0$ and away from the band-edge points.
- (b) Find the relationship between the expansion coefficients b_n and the Fourier expansion coefficients for the periodic potential $V(x)$ for this case. Also, obtain an analytic expression for the dispersion relation (the relationship between the allowed particle energies and the crystal momentum k) for values of the crystal momentum away from the band-edge points.
- (c) How will the results from parts (a-c) change if the crystal momentum approaches the band edge points $k_n = \pm n\pi/a$? What is the appropriate approximate expression for the wavefunction in this case? Evaluate the dispersion relation in the vicinity of the band edge points and discuss the overall energy-wavevector dispersion relation in the free-electron approximation.
3. In the free-electron approximation, discussed in problem 2, it was assumed that the potential energy of the electron is small compared to its total energy. The atoms are assumed to be very close to each other, so that there is significant overlap between the wavefunctions for the electrons associated with neighboring atoms. This leads to wide energy bands and very narrow energy gaps. The tight-binding approximation proceeds from the opposite limit, i.e. it assumes that the potential energy of the electron accounts for nearly all of the total energy. The atoms are assumed to be very far apart so that the wavefunctions for the electrons associated with neighboring atoms overlap only to a small extent. A brief description of the tight-binding method is given below:

If the potential function associated with an isolated atom is $V_0(\mathbf{r})$, then the solution of the Schrödinger equation

$$\hat{H}_0 \psi_0(\mathbf{r}) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_0(\mathbf{r}) \right] \psi_0(\mathbf{r}) = E_0 \psi_0(\mathbf{r}), \quad (3.1)$$

describes the electronic wavefunctions of the atom. If the ground-state wavefunction is not much affected by the presence of the neighboring atoms, then the crystal wavefunction is given by:

$$\psi(\mathbf{r}) = \sum_n e^{i\mathbf{k}_n \cdot \mathbf{r}} \psi_0(\mathbf{r} - \mathbf{r}_n), \quad (3.2)$$

and the periodic potential is represented as

$$V(\mathbf{r}) = \sum_n V_0(\mathbf{r} - \mathbf{r}_n), \quad (3.3)$$

where \mathbf{r}_n is a vector from some reference point in space to a particular lattice site. Now, if we express the potential energy term in the total Hamiltonian of the system as

$$V(\mathbf{r}) = V_0(\mathbf{r} - \mathbf{r}_n) + V(\mathbf{r}) - V_0(\mathbf{r} - \mathbf{r}_n) = V_0(\mathbf{r} - \mathbf{r}_n) + H'(\mathbf{r}), \quad (3.4)$$

it is rather straightforward to show that the expectation value of the energy of the system is given by

$$E = E_0 + \frac{1}{N} \sum_m e^{-i\mathbf{k} \cdot \mathbf{r}_m} \int dV \psi_0^*(\mathbf{r} - \mathbf{r}_m) [V(\mathbf{r}) - V_0(\mathbf{r})] \psi_0(\mathbf{r}). \quad (3.5)$$

where N is the number of atoms in the crystal.

- (a) Complete the derivation that leads to the result given in (3.5).
- (b) If we assume that the atomic wavefunctions are spherically symmetric (*s*-type), show that in the case then the nearest-neighbor interaction are only taken into account, the energy of the system for simple cubic lattice is of the form

$$E = E_0 - \alpha - 2\beta [\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]. \quad (3.6)$$

Identify the meaning of the terms α and β in the result given in (3.6). What is the approximate form of the dispersion relation for an electron moving in the x -direction with momentum $k_x \ll \pi/a$.

- (c) Find the dispersion relation for an *s*-band in the tight-binding approximation for a body-centered and face-centered cubic crystal in the tight-binding approximation, considering overlap of nearest-neighbor wavefunctions only.
- (d) Plot the form of the constant energy surfaces for several energies within the zone. Show that these surfaces are spherical for energies near the bottom of the band.
- (e) Show that $\mathbf{n} \cdot \nabla_{\mathbf{k}} E$ vanishes on the zone boundaries.