

Series – Semiconductor physics and fundamentals of electronic devices

Academic year 2016-2017 – 1st semester

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Series 2 – Brillouin zone, periodic potentials in one dimension (Kronig-Penney model)

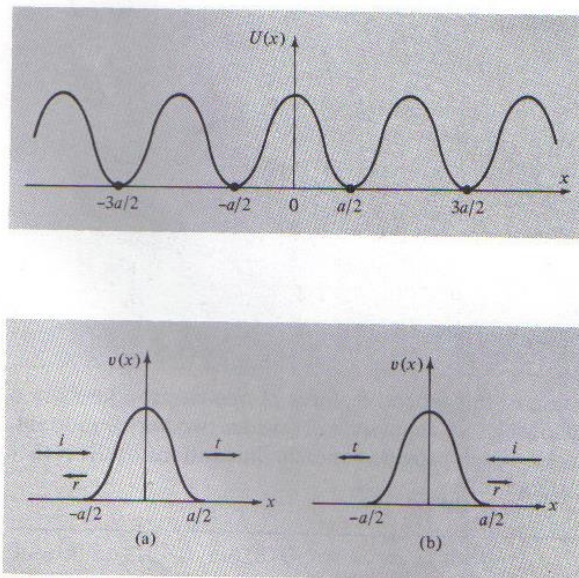
Exercise 1: Introduction to Brillouin zones

- 1- Consider a square two-dimensional reciprocal lattice. Draw the first and the second Brillouin zone of this lattice.
- 2- What is the number of first and second nearest neighbors of a square lattice in real space?
- 3- Solve the same questions in the specific case of a two-dimensional hexagonal (honeycomb) lattice.

Nota bene: The first Brillouin zone is delimited by the midperpendicular of the first points of the reciprocal lattice. Note that any point can be chosen to be the origin of this lattice.

Exercise 2: Periodic potentials in one dimension (Kronig-Penney model). Problem adapted from *Solid State Physics* by N.W. Ashcroft and N.D. Mermin (Saunders College Publishing, Orlando, 1976).

Consider a one-dimensional periodic potential $U(x)$ where the ions reside at the minima of U , which we take to define the zero of energy. We choose to view the periodic potential as a superposition of potential barriers $v(x)$ of width a , centered at the points $x = \pm na$ (**Fig. 1**):



$$U(x) = \sum_{n=-\infty}^{+\infty} v(x - na). \quad (1)$$

The term $v(x-na)$ represents the potential barrier against an electron tunneling between the ions on opposite sides of the point na . For simplicity we assume that $v(x) = v(-x)$, but we make

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no other assumptions about v , so the form of the periodic potential U is quite general. The band structure of the one-dimensional solid can be expressed quite simply in terms of the

properties of an electron in the presence of a single-barrier potential $v(x)$. Consider therefore an electron incident from the left on the potential barrier $v(x)$ with energy $\varepsilon = \hbar^2 k^2 / 2m$ (Note that in this problem the wave vector k is a continuous variable and has nothing to do with the reciprocal lattice). Since $v(x) = 0$ when $|x| \geq a/2$, in these regions the wave function $\psi_l(x)$ will have the form (see **Fig. 1**):

$$\psi_l(x) = e^{ikx} + re^{-ikx}, \quad x \leq -a/2, \quad (2)$$

$$\psi_l(x) = te^{ikx}, \quad x \geq a/2. \quad (3)$$

The transmission and reflection coefficients t and r give the probability amplitude that the electron will tunnel through or be reflected from the barrier. They depend on the incident wave vector k in a manner determined by the detailed features of the barrier potential v . However, one can deduce many properties of the band structure of the periodic potential U by appealing only to very general properties of t and r . Because v is even, $\psi_r(x) = \psi_l(-x)$ is also a solution to the Schrödinger equation with energy ε . From (2) and (3), it follows that $\psi_r(x)$ has the form:

$$\psi_r(x) = te^{-ikx}, \quad x \leq -a/2, \quad (4)$$

$$\psi_r(x) = e^{-ikx} + re^{ikx}, \quad x \geq a/2. \quad (5)$$

Since $\psi_l(x)$ and $\psi_r(x)$ are two independent solutions to the single-barrier Schrödinger equation with the same energy, any other solution with that energy will be a linear combination of these two. In particular, since the crystal Hamiltonian is identical to that for a single ion in the region $-a/2 \leq x \leq a/2$, any solution to the crystal Schrödinger equation with energy ε must be a linear combination of $\psi_l(x)$ and $\psi_r(x)$ in that region:

$$\psi(x) = A\psi_l(x) + B\psi_r(x), \quad |x| \geq a/2. \quad (6)$$

Now Bloch's theorem asserts that ψ can be chosen to satisfy:

$$\psi(x+a) = e^{iGa}\psi(x), \quad (7)$$

for suitable G . Differentiating (7) we also find that $\psi' = d\psi/dx$ satisfies:

$$\psi'(x+a) = e^{iGa}\psi'(x). \quad (8)$$

1. By imposing the conditions (7) and (8) at $x = -a/2$, and using (2) to (6), show that the energy of the Bloch electron is related to its wave vector G by:

$$\cos Ga = \frac{t^2 - r^2}{2t} e^{ika} + \frac{1}{2t} e^{-ika}, \quad \varepsilon = \frac{\hbar^2 k^2}{2m}. \quad (9)$$

Verify that this gives the right answer in the free electron case ($v \equiv 0$).

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We write the complex number t in terms of its magnitude and phase:

$$t = |t|e^{i\delta}. \quad (10)$$

More precisely, the real number δ is known as the phase shift, since it specifies the change in phase of the transmitted wave relative to the incident one. In addition, electron conservation requires that the probability of transmission plus the probability of reflection be unity:

$$1 = |t|^2 + |r|^2. \quad (11)$$

It is also possible to show that r must have the form:

$$r = \pm i|r|e^{i\delta}, \quad (12)$$

where δ is the same as in (10).

2. Show as a consequence of (9), (11) and (12) that the energy and wave vector of the Bloch electron are related by:

$$\frac{\cos(ka + \delta)}{|t|} = \cos Ga, \quad \varepsilon = \frac{\hbar^2 k^2}{2m}. \quad (13)$$

Since $|t|$ is always less than one, but approaches unity for large k (the barrier becomes increasingly less effective as the incident energy grows), the left side of (13) plotted against k has the structure depicted in **Fig. 2**. For a given G , the allowed values of k (and hence the allowed energies $\varepsilon(G) = \frac{\hbar^2 k^2}{2m}$) are given by the intersection of the curve in **Fig. 2** with the horizontal line of height $\cos(Ga)$. Note that values of k in the neighborhood of those satisfying:

$$ka + \delta = n\pi \quad (14)$$

give $|\cos(ka + \delta)|/|t| > 1$, and are therefore not allowed for any G . The corresponding regions of energy are the energy gaps. If δ is a bounded function of k (as is generally the case), then there will be infinitely many regions of forbidden energy, and also infinitely many regions of allowed energies for each value of G .

3. Draw the band diagram (qualitative picture) deduced from **Fig. 2** (energy versus G).
4. Suppose the barrier is very weak (so that $|t| \approx 1, |r| \approx 0, \delta \approx 0$). What is the width of the gap ε_{gap} near $k = \frac{n\pi}{a}$?

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5. Suppose now the barrier is very strong (so that $|t| \approx 0, |r| \approx 1$). Show that the allowed bands of energies are then very narrow, with widths: $\varepsilon_{\max} - \varepsilon_{\min} = o(|t|)$. (15)

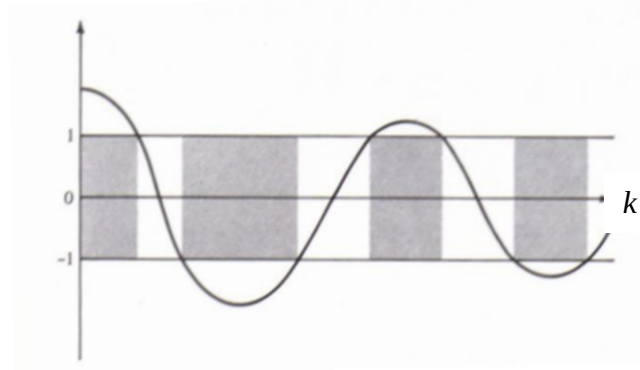


Figure 2: Characteristic form of (13, left-hand side). Because $|t(k)|$ is always less than unity, (13) will exceed unity in magnitude in the neighborhood of solutions to $ka + \delta(k) = n\pi$. Equation (13) can be satisfied for real G if and only if the function is less than unity in magnitude. Consequently there will be allowed (unshaded) and forbidden (shaded) regions of G (and therefore of $\varepsilon(G) = \frac{\hbar^2 k^2}{2m}$).