

Solids II

Lecture 34

Physics 342 Quantum Mechanics I

Friday, April 23rd, 2010

34.1 Lattice Potential

A refinement of the free electron gas introduces fixed nuclei – we imagine that the electrons move around under the attractive influence of the atomic nuclei fixed on some grid. To understand the basic physics of the model (originally introduced by Kronig-Penney), we can take a simple one-dimensional, periodic train of delta spikes.

Consider a set of equally spaced delta spikes, separated by a distance ℓ , and given some scale α , so that each contributes $V_\delta = \alpha \delta(x - j\ell)$ to the potential ($j \in \mathbb{Z}$). We assume that the potential continues “forever” (i.e. that there are a large number of nuclei), and that the wave-function must be bounded in magnitude (not going to infinity at spatial infinity). The potential is shown in Figure 34.1.

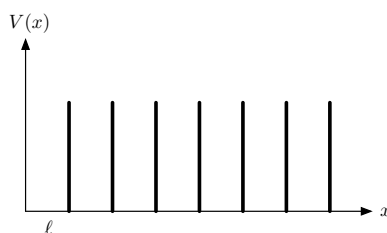


Figure 34.1: An infinite string of Dirac spikes separated by equal distance ℓ .

The wave function can be thought of as a piecewise function – in between each spike, we must satisfy $-\frac{\hbar^2}{2m} \psi''(x) = E \psi(x)$, and we know the solution

for the j^{th} wave function (the one defined for $j\ell \leq x \leq (j+1)\ell$):

$$\psi_j = A_j \cos(kx) + B_j \sin(kx) \quad k^2 \equiv \frac{2mE}{\hbar^2} \quad (34.1)$$

From the boundary conditions appropriate to the delta spike, we can relate the solution ψ_{j+1} to ψ_j :

$$\psi_j((j+1)\ell) = \psi_{j+1}((j+1)\ell) \quad \psi'_{j+1}((j+1)\ell) - \psi'_j((j+1)\ell) = \frac{2m\alpha}{\hbar^2} \psi_j((j+1)\ell). \quad (34.2)$$

If we think of a local $x_j = x - j\ell$ that goes, in each “cell” from $0 \rightarrow \ell$, then we can write the connection between any two cells as:

$$\begin{aligned} \psi_j(x_j = \ell) &= \psi_{j+1}(x_{j+1} = 0) \\ \psi'_{j+1}(x_{j+1} = 0) - \psi'_j(x_j = \ell) &= \frac{2m\alpha}{\hbar^2} \psi_{j+1}(x_{j+1} = 0). \end{aligned} \quad (34.3)$$

In terms of the coefficients, we have:

$$\begin{aligned} A_{j+1} &= A_j \cos(k\ell) + B_j \sin(k\ell) \\ k B_{j+1} - k B_j \cos(k\ell) + k A_j \sin(k\ell) &= \frac{2m\alpha}{\hbar^2} A_{j+1} \end{aligned} \quad (34.4)$$

and we can write this in terms of the transfer matrix:

$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = \underbrace{\begin{pmatrix} \cos(k\ell) & \sin(k\ell) \\ \frac{2m\alpha}{\hbar^2 k} \cos(k\ell) - \sin(k\ell) & \frac{2m\alpha}{\hbar^2 k} \sin(k\ell) + \cos(k\ell) \end{pmatrix}}_{\equiv \mathbb{M}} \begin{pmatrix} A_j \\ B_j \end{pmatrix}. \quad (34.5)$$

Now we can move directly to the solution ψ_{j+1} by multiplication:

$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = \mathbb{M}^j \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \quad (34.6)$$

and this multiplication is dominated by the behavior of the eigenvalues of \mathbb{M} – if the eigenvalues have magnitude > 1 , it will diverge from some initial set of coefficients, to infinity. So to get a well-behaved wave-function, we must have both of the eigenvalues of \mathbb{M} bounded in magnitude by 1.

The eigenvalues of this two-by-two matrix are easy to write out:

$$\lambda_{\pm} = \cos(k\ell) + \frac{m\alpha}{\hbar^2 k} \sin(k\ell) \pm \sqrt{\sin(k\ell) \left(\frac{2m\alpha}{\hbar^2 k} \cos(k\ell) + \left(\frac{m^2 \alpha^2}{\hbar^4 k^2} - 1 \right) \sin(k\ell) \right)}. \quad (34.7)$$

Without worrying about the complex magnitude, suppose we set each of these separately equal to a function of k , $f_{\pm}(k)$ – then we can solve for $f_+(x) + f_-(x)$ by substitution

$$f_+(x) + f_-(x) = 2 \cos(k\ell) + \frac{2m\alpha}{\hbar^2 k} \sin(k\ell). \quad (34.8)$$

Our requirement is that the functions $f_{\pm}(k)$ be, individually, less than or equal to one in absolute value, so that the infinite matrix multiplication converges (to ± 1 or 0), and this gives us a constraint on the energy $k = \frac{\sqrt{2mE}}{\hbar}$ – we have admissible solutions only when

$$\left| \cos(k\ell) + \frac{m\alpha}{\hbar^2 k} \sin(k\ell) \right| \leq 1. \quad (34.9)$$

Defining the unitless constants $\frac{m\alpha\ell}{\hbar^2 k} \equiv \beta$, and $k\ell = z$, our requirement is

$$\left| \cos(z) + \frac{\beta}{z} \sin(z) \right| \leq 1. \quad (34.10)$$

Now for the physical point – looking at the solutions to this inequality for various β (delta strengths), we see that there are “gaps” in the energy, where there is no valid solution for k , and “bands” where k varies continuously. As an example, take $\beta = 2$ – we show the value of the left-hand side of (34.10), together with a function that is 1 when there are allowed solutions, 0 otherwise in Figure 34.2.

While this is a simple one-dimensional picture, the idea carries over to two and three dimensions. In our electron gas model, there was a continuum of energies allowed, but when we introduce a periodic potential (due to whatever mechanism), we find that there are “continuum” regions, where electrons can gain energy (filling the band), and then gaps, where we need to add some amount of energy to get an electron through to the next band. Materials with significant gap structure are insulators, difficult to get electrons moving (you have to input energy in a filled band to get the electron to cross it) – materials where a band is relatively unfilled are conductors – it takes very little energy to move an electron (since there is a local continuum of energies for it to exist in).

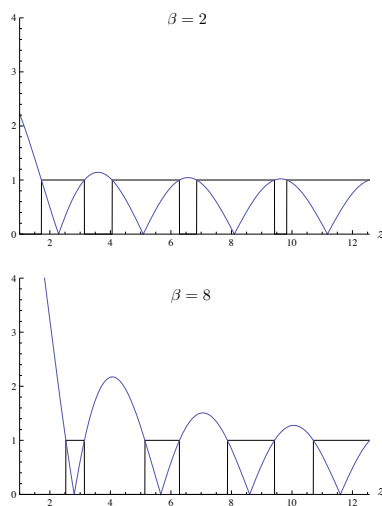


Figure 34.2: The left-hand side of (34.10) and a step function to show the allowed regimes for $\beta = 2, 8$.

Homework

Reading: Griffiths, pp. 224–229.

Problem 34.1

Griffiths 5.20. Running the Dirac comb argument for delta wells.