Lecture 32: Transfer Matrices for Periodic Potentials

Monday, November 04, 2019

From the last lecture, we found that a potential with $V(x+a) = V(x)$ gave solutions of the form

$$\psi_q(x) = e^{\imath qx} U_q(x)$$

where $U_q(x+a) = U_q(x)$. Suppose we were in a region where $V(x) = 0$. We would then have left and right-going solutions like

$$\psi = A_0 e^{\imath kx} + B_0 e^{-\imath kx}$$

If we imagine the potential as having some shape which we are transmitting through or reflecting against centered about $x = 0$, we can say that to the left of this potential we have the above solution and to the right of the potential we have a similar solution

$$\psi = A_1 e^{\imath kx} + B_1 e^{-\imath kx}$$

Now we need to find the relationship between each coefficient and the coefficient in the next valley:

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = M \begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix}$$

where

$$M = \begin{bmatrix} \gamma & \delta \\ \delta^* & \gamma^* \end{bmatrix}$$

where $|\gamma|^2 - |\delta|^2 = 1$.

By the Bloch theorem from last lecture, we had $\psi(x+a) = e^{\imath qa}\psi(x)$, so

$$A_{n+1} e^{\imath k(x+a)} + B_{n+1} e^{-\imath k(x+a)} = e^{\imath qa} \left(A_n e^{\imath kx} + B_n e^{-\imath kx} \right)$$

so

$$e^{\imath qa} \begin{bmatrix} A_n \\ B_n \end{bmatrix} = \begin{bmatrix} e^{\imath ka} & 0 \\ 0 & e^{-\imath ka} \end{bmatrix} \underbrace{\begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix}}_{M^{-1} \begin{bmatrix} A_n \\ B_n \end{bmatrix}}$$

Example. Let's look at a specific example of periodic δ-functions.

$$V(x) = \sum_{n=-\infty}^{\infty} \left(\frac{\hbar^2}{2m} \right) g\delta(x - na)$$

By continuity at $x = 0$, we have

$$A_0 \left[1 - e^{\imath(q-k)a} \right] + B_0 \left[1 - e^{\imath(q+k)a} \right] = 0$$

and by continuity of the derivative at $x = 0$,

$$A_0 \left[g + \imath k \left(1 - e^{\imath(q-k)a} \right) \right] + B_0 \left[g - \imath k \left(1 - e^{\imath(q+k)a} \right) \right] = 0$$

We can't solve this system of equations since there are too many unknowns, but we can find a relation which will give us a relation for the allowed energy values. Note that the system can be put into matrix form over A_0 and B_0 and the determinant of this matrix is zero. Solving this gives

$$\cos(qa) = \cos(ka) + \frac{\alpha}{2ka} \sin(ka) = F(ka)$$

We won't allow solutions where $|F(ka)| > 1$, since this would require an imaginary q, which would cause diverging solutions in the original wave function. We can find allowed values of k by choosing values of q, for example, finding solutions of

$$\cos(k_0 a) + \frac{\alpha}{2k_0 a} \sin(k_0 a) = 1$$

when $q = 0$. These allowed and forbidden regions correspond to bands in k, which means there are allowed and forbidden bands in energy as well, since $k \sim \sqrt{E}$.

Near the band edge where $q \approx 0$,

$$\begin{aligned} F(qa) &= F(k_a) + (k - k_0)aF'(k_0 a) + \cdots \\ &= 1 + (k - k_0)aF'(k_0 a) \approx 1 - \frac{(qa)^2}{2} \end{aligned}$$

so

$$k - k_0 = \frac{q^2 a}{2|F'(k_0 a)|}$$

We can also expand this in E:

$$\begin{aligned} E(k) = \frac{\hbar^2}{2mc^2} &= E(k_0) + \frac{\hbar^2(k^2 - k_0^2)}{2m} \\ &\approx E(k_0) + \frac{\hbar^2 k(k - k_0)}{2m} \\ &\approx E_0 + \frac{\hbar^2 k_0}{m}\frac{q^2 a}{2|F'|} \end{aligned}$$

Plotting this band structure as a function of q gives us: ◇

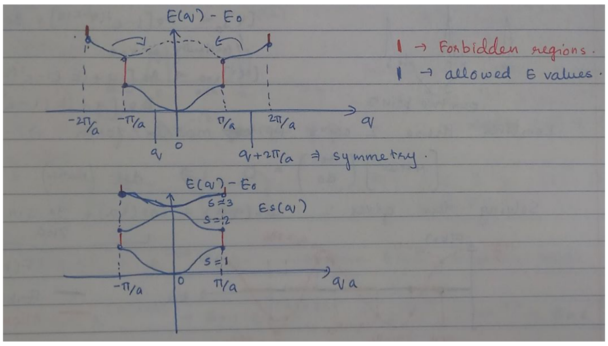

Figure 0.0.1: Band Structure for Dirac Comb