Kronig - Penney model in reciprocal space

$$U(x) = 2\sum_{G\geq 0}' U_G \cos(Gx) = Aa\sum_s' \delta(x-sa)$$

A: constant

a: lattice constant

s : integer $0 < s < \frac{1}{a}$

Apply PBC method over a ring of unit length containing 1/a atoms.

$$U(x) = \sum_G' U_G e^{iGx} = Aa\sum_s' \delta(x-sa)$$

$$U_G = \int_0^1 U(x)\, e^{-iGx}\, dx$$

$$= Aa\sum_s \int_0^1 \delta(x-sa)\, e^{-iGx}\, dx$$

$$= Aa\sum_s e^{-iGsa}$$

G : reciprocal vector

$G = \frac{2\pi}{a} n$ with n an integer

$$= Aa\sum_s e^{-i2\pi ns}$$

$Ga = 2\pi n$

$s \in \mathbb{Z}$

$$e^{-i2\pi ns} = (e^{-i2\pi})^{ns} = 1^{ns}$$

$$U_G = Aa\sum_{s=0}^{1/a} 1 = Aa\frac{1}{a} = \boxed{A = U_G}$$

The central equation becomes

$$(\lambda_k - E)\, C_k + \sum_G' U_G\, C_{k-G} = 0 \qquad \lambda_k = \frac{\hbar^2 k^2}{2m}$$

$G = \frac{2\pi n}{a}$

$$(\lambda_k - E) C_k + A \sum_n' C_{k-\frac{2\pi n}{a}} = 0$$

We solutions for the coefficients C_k!

Let's define

$$f(k) = \sum_n' C_{k-\frac{2\pi n}{a}}$$

$$(\lambda_k - E) C_k + A f(k) = 0 \rightarrow C_k = \frac{A f(k)}{E - \lambda_k} \qquad \lambda_k = \frac{\hbar^2 k^2}{2m}$$

$$C_k = \frac{A f(k)}{E - \frac{\hbar^2 k^2}{2m}} = \frac{A f(k)}{\frac{\hbar^2}{2m}\left(\frac{2mE}{\hbar^2} - k^2\right)} = \frac{2m}{\hbar^2} \frac{A f(k)}{\left(\frac{2mE}{\hbar^2} - k^2\right)}$$

The sum in $f(k)$ is over all integers

$$f(k) = f(k - 2\pi n/a)$$

So we can write

$$C_{k-\frac{2\pi n}{a}} = \frac{2m}{\hbar^2} \frac{A f(k)}{\left(\frac{2mE}{\hbar^2}\right) - \left(k - \frac{2\pi n}{a}\right)^2}$$

$$\sum_n C_{k-\frac{2\pi n}{a}} = \sum_n' \frac{2m}{\hbar^2} \frac{A f(k)}{\left(\frac{2mE}{\hbar^2}\right) - \left(k - \frac{2\pi n}{a}\right)^2}$$

$$f(k) = \frac{2m}{\hbar^2} A f(k) \sum_n' \frac{1}{\left(\frac{2mE}{\hbar^2}\right) - \left(k - \frac{2\pi n}{a}\right)^2}$$

$$\frac{\hbar^2}{2mA} = \sum_n' \frac{1}{\left(\frac{2mE}{\hbar^2}\right) - \left(k - \frac{2\pi n}{a}\right)^2}$$

Let's define $Q^2 = \frac{2mE}{\hbar^2}$

$$\sum_n' \frac{1}{Q^2 - \left(k - \frac{2\pi n}{a}\right)^2} = \sum_n' \frac{1}{\left[Q - \left(k - \frac{2\pi n}{a}\right)\right]\left[Q + \left(k - \frac{2\pi n}{a}\right)\right]} = \otimes$$

$$a^2 - b^2 = (a+b)(a-b)$$

$$\frac{1}{(a+b)(a-b)} = \frac{1}{2a}\left[\frac{1}{a-b} + \frac{1}{a+b}\right] \qquad a = Q \quad b = k - \frac{2\pi n}{a}$$

$$\otimes = \sum_n' \frac{1}{2Q}\left\{\frac{1}{Q - \left(k - \frac{2\pi n}{a}\right)} + \frac{1}{Q + \left(k - \frac{2\pi n}{a}\right)}\right\} = \otimes$$

$$Q - k + \frac{2\pi n}{a} = \frac{2}{a}\left\{\frac{a}{2}(Q-k) + n\pi\right\}$$

$$Q + k - \frac{2\pi n}{a} = \frac{2}{a}\left\{\frac{a}{2}(Q+k) - n\pi\right\} = -\frac{2}{a}\left\{-\frac{a}{2}(Q+k) + n\pi\right\}$$

$$\otimes = \sum_n' \frac{1}{2Q}\left\{\frac{1}{\frac{2}{a}\left[\frac{a}{2}(Q-k) + n\pi\right]} - \frac{1}{\frac{2}{a}\left[-\frac{a}{2}(Q+k) + n\pi\right]}\right\}$$

$$= \sum_n' \frac{1}{2Q}\frac{a}{2}\left\{\frac{1}{n\pi + \frac{a}{2}(Q-k)} - \frac{1}{n\pi - \frac{a}{2}(Q+k)}\right\}$$

$$\cot(x) = \frac{\cos(x)}{\sin(x)} = \sum_n' \frac{1}{n\pi + x} \qquad \cot(-x) = -\cot(x)$$

$$= \frac{a}{4Q}\left\{\cot\left[\frac{a}{2}(Q-k)\right] - \cot\left[-\frac{a}{2}(Q+k)\right]\right\}$$

$$= \frac{a}{4Q}\left\{\cot\left[\frac{a}{2}(Q-k)\right] + \cot\left[\frac{a}{2}(Q+k)\right]\right\}$$

$$\cot(\alpha) + \cot(\beta) = \frac{\cot(\alpha)\cot(\beta) + 1}{\cot(\alpha+\beta)}$$

$$= \frac{a}{4Q}\,\frac{\cot\left[\frac{a}{2}(Q-k)\right]\cot\left[\frac{a}{2}(Q+k)\right] + 1}{\cot(aQ)} = \otimes$$

Here:

Use the following

$$\cot(\alpha) = \frac{\cos(\alpha)}{\sin(\alpha)}$$

$$\cos(\alpha+\beta) = \cos\alpha\cos\beta - \sin\alpha\sin\beta$$

$$\cos(\alpha-\beta) = \cos\alpha\cos\beta + \sin\alpha\sin\beta$$

$$\sin\alpha\sin\beta = \cos(\alpha-\beta) - \cos(\alpha+\beta)$$

$$* = \frac{a}{4Q} \frac{\sin(Qa)}{\cos(ka) - \cos(Qa)}$$

$$= \frac{a^2}{4} \frac{\sin(Qa)}{Qa} \frac{1}{\cos(ka) - \cos(Qa)} = \frac{\hbar^2}{2mA}$$

$$1 = \frac{2mA}{\hbar^2} \frac{a^2}{4} \frac{\sin(Qa)}{Qa} \frac{1}{\cos(ka) - \cos(Qa)}$$

$$\cos(ka) - \cos(Qa) = \frac{2mA}{\hbar^2} \frac{a^2}{4} \frac{\sin(Qa)}{Qa}$$

$$\boxed{\cos(ka) = \cos(Qa) + \frac{2mA}{\hbar^2} \frac{a^2}{4} \frac{\sin(Qa)}{Qa}}$$

This agrees with the result for the Kronig-Penney model with $P = \frac{mAa}{2\hbar^2}$

Approximate solution near the zone boundary

$U_G \ll$ Kinetic energy at the edge of the BZ.

$$k^2 = \left(\frac{1}{2}G\right)^2 \qquad (k-G)^2 = \left(\frac{1}{2}G - G\right)^2$$
$$= \left(-\frac{1}{2}G\right)^2 = \left(\frac{1}{2}G\right)^2$$

At the boundary K_E of the two waves with $k = \pm\frac{1}{2}G$ is equal.

If the coefficient $C_{G/2}$ in important in the expansion, the $C_{-G/2}$ is also importent

In the central eq.; assuming that we only have $C_{-G/2}$ and $C_{G/2}$

$$\lambda_k = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 G^2}{8m} \quad \text{for both} \quad k = \pm\frac{G}{2}$$
$$= \lambda$$

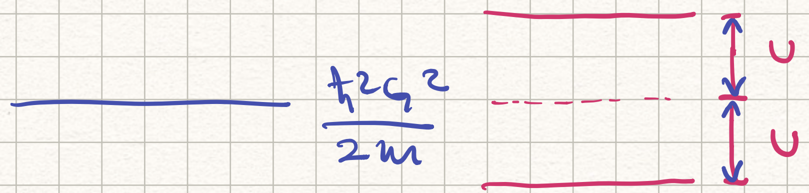
$$(\lambda - E)\, C_{G/2} + U C_{-G/2} = 0$$

$$(\lambda - E)\, C_{-G/2} + U C_{G/2} = 0$$

The are nontrivial solutions of

$$\det \begin{pmatrix} \lambda - E & U \\ U & \lambda - E \end{pmatrix} = 0 = (\lambda - E)^2 - U^2$$

$$E = \lambda \pm U$$
$$= \frac{\hbar^2 G^2}{8m} \pm U$$



The potential $U(x) = 2U\cos(Gx)$ has created an energy gap of $2U$ at the zone boundary

The ratio of the coefficients is obtaine as

$$(\lambda - E)\, C_{G/2} + U C_{-G/2} = 0$$
$$(\lambda - E)\, C_{-G/2} + U C_{G/2} = 0$$

$$C_{G/2} = \frac{U}{E-\lambda} C_{-G/2} \Rightarrow \frac{C_{G/2}}{C_{-G/2}} = \frac{U}{E-\lambda}$$

$$E = \lambda \pm U \Rightarrow E - \lambda = \pm U$$

$$\frac{C_{G/2}}{C_{-G/2}} = \frac{U}{\pm U} = \pm 1$$

At ZB the wave function is

$$\psi(x) = A\left(e^{iGx/2} \pm e^{-iGx/2}\right)$$

: it is a standing wave

Near the boundary

we use a two-component approximation to find $\psi(x)$ near the ZB:

$$\psi(x) = C_k e^{ikx} + C_{k-G} e^{i(k-G)x}$$

The central eq.

$$(\lambda_k - E) C_k + U C_{k-G} = 0$$

$$\lambda_k = \frac{\hbar^2 k^2}{2m}$$

$$(\lambda_{k-G} - E) C_{k-G} + U C_k = 0$$

The solutions exist

$$(\lambda_k - E)(\lambda_{k-G} - E) - U^2 = 0$$

$$E^2 - E(\lambda_k + \lambda_{k-G}) + \lambda_k \lambda_{k-G} - U^2 = 0$$

$$E = \frac{1}{2}(\lambda_k + \lambda_{k-G}) \pm \frac{1}{2}\sqrt{(\lambda_k + \lambda_{k-G})^2 - 4\lambda_k \lambda_{k-G} + 4U^2}$$

$$= \frac{1}{2}(\lambda_k + \lambda_{k-G}) \pm \sqrt{\frac{1}{4}(\lambda_k - \lambda_{k-G})^2 + U^2}$$

Each root $\Rightarrow$ energy band.

$k = \frac{1}{2}G + \tilde{k}$ $\qquad$ $\tilde{k}$ we take as very small

$$\lambda_k = \frac{\hbar^2 k^2}{2m}$$

$$\lambda_{k-G} = \frac{\hbar^2}{2m}(k-G)^2 = \frac{\hbar^2}{2m}(k^2 + G^2 - 2kG)$$

$$\lambda_k + \lambda_{k-G} = \frac{\hbar^2}{2m}(2k^2 + G^2 - 2kG)$$

$\tilde{k} = k - \frac{1}{2}G$ $\qquad$ $\tilde{k}^2 = k^2 + \frac{1}{4}G^2 - kG$

$$2\tilde{k}^2 = 2k^2 + \frac{1}{2}G^2 - 2kG$$

$$2\tilde{k}^2 - \frac{1}{2}G^2 = 2k^2 - 2kG$$

$$\lambda_k + \lambda_{k-G} = \frac{\hbar^2}{2m}\left(2\tilde{k}^2 - \frac{1}{2}G^2 + G^2\right)$$

$$= \frac{\hbar^2}{2m}\left(2\tilde{k}^2 + \frac{1}{2}G^2\right)$$

$$\frac{1}{2}(\lambda_k + \lambda_{k-G}) = \frac{\hbar^2}{2m}\left(\tilde{k}^2 + \frac{1}{4}G^2\right)$$

$$\lambda = \frac{\hbar^2 G^2}{8m}$$

$$(\lambda_k - \lambda_{k-G})^2 = 4\cdot\left(4\lambda\frac{\hbar^2\tilde{k}^2}{2m}\right)$$

Replacing everything

$$E = \frac{\hbar^2}{2m}\left(\tilde{k}^2 + \frac{1}{4}G^2\right) \pm \sqrt{4\lambda\frac{\hbar^2\tilde{k}^2}{2m} + U^2}$$

$$= \frac{\hbar^2}{2m}\left(\tilde{k}^2 + \frac{1}{4}G^2\right) \pm U\sqrt{\frac{4\lambda}{U^2}\frac{\hbar^2\tilde{k}^2}{2m} + 1}$$

In the limit $\frac{4\lambda}{U^2}\frac{\hbar^2\tilde{k}^2}{2m} << 1$

$$\sqrt{1+x^2} \approx 1 + \frac{1}{2}x^2$$

$$E = \frac{\hbar^2}{2m}\left(\tilde{k}^2 + \frac{1}{4}G^2\right) \pm U\left[1 + \frac{1}{2}\frac{4\lambda}{U^2}\frac{\hbar^2\tilde{k}^2}{2m}\right]$$

$$= \frac{\hbar^2}{2m}\left(\tilde{k}^2 + \frac{1}{4}G^2\right) \pm U\left[1 + \frac{\hbar^2\tilde{k}^2\lambda}{mU^2}\right]$$

$$= \frac{\hbar^2 G^2}{8m} \pm U + \frac{\hbar^2\tilde{k}^2}{2m} \pm \frac{\hbar^2\tilde{k}^2}{2m}\frac{2\lambda}{U}$$

$$E = \underbrace{\left[\lambda \pm U\right]}_{\text{Energy at the edge of the boundary}} + \underbrace{\frac{\hbar^2\tilde{k}^2}{2m}\left[1 \pm \frac{2\lambda}{U}\right]}_{\text{Correction for being away from the edge}}$$

Energy at the edge of the boundary

Correction for being away from the edge