Transmission matrix (periodic potentials)

Recall Bloch Theorem: $V(x+a) = V(x) \Rightarrow \begin{cases} 1.\ \varphi(x+a) = e^{iqa}\varphi(x) \\ 2.\ \varphi_q(x) = e^{iqx}u_q(x) \end{cases}$

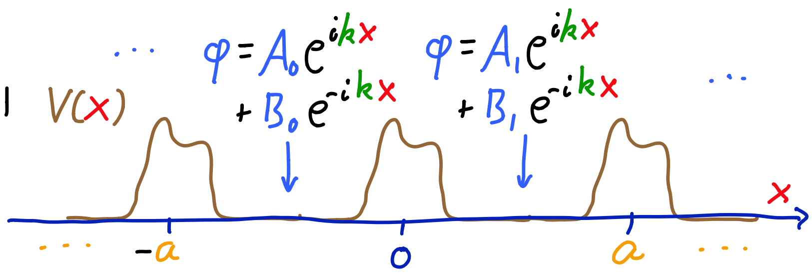
Schrödinger approach

$$\left\{ \frac{p^2}{2m} + V(x) \right\} e^{iqx} u(x) = E\, e^{iqx} u(x)$$

Alternative approach

piecewise zero potential

$k = \sqrt{2mE/\hbar^2}$



$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = M(k) \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} \qquad M = \begin{pmatrix} \gamma & \delta \\ \delta^* & \gamma^* \end{pmatrix} \qquad |\gamma|^2 - |\delta|^2 = 1$$

But: $\varphi(x+a) = e^{iqa}\varphi(x) \Rightarrow A_{n+1} e^{iq(x+a)} + B_{n+1} e^{-iq(x+a)}$

$$= e^{iqa}\left(A_n e^{iqx} + B_n e^{-iqx}\right)$$

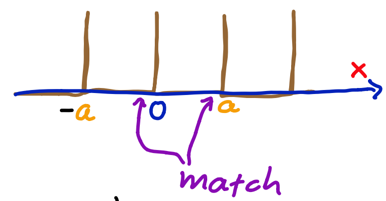
$$e^{iqa} \begin{pmatrix} A_n \\ B_n \end{pmatrix} = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \underbrace{\begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} M^{-1}(k)}_{\tilde{M}(k)} \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

$\begin{pmatrix} A_n \\ B_n \end{pmatrix}$ is eigenvector of $\tilde{M}(k)$ with eigenvalue e^{iqa}

$\Rightarrow$ functional relationship $q \to k \to E(q)$

δ-function potential

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



Let
$$\varphi(x)=\begin{cases} A_0 e^{ikx}+B_0 e^{-ikx} & (-a<x<0)\\ A_1 e^{ikx}+B_1 e^{-ikx} & (0<x<a)\end{cases}$$

Periodicity: $\varphi(x+a)=e^{iqa}\varphi(x) \Rightarrow A_1 e^{ika}=A_0 e^{iqa},\quad B_1 e^{-ika}=B_0 e^{iqa}$

$$A_0 - A_1 \qquad + \qquad B_0 - B_1$$

φ Continuity at $x=0$: $\quad A_0\left[1-e^{i(q-k)a}\right]+B_0\left[1-e^{i(q+k)a}\right]=0$

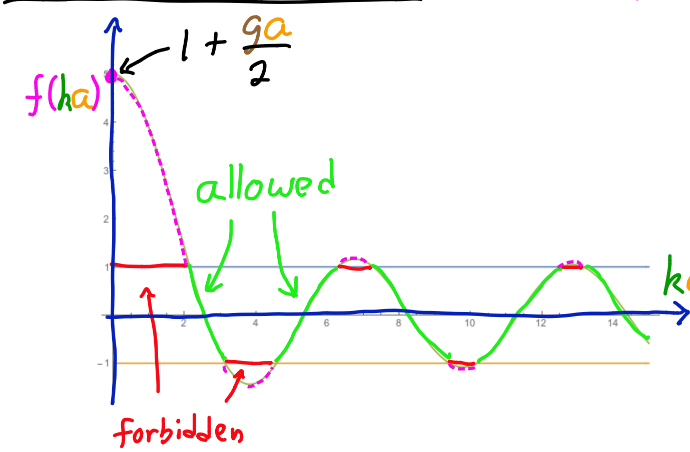
φ' discontinuity at $x=0$: $\quad A_0\left[g+ik\left(1-e^{i(q-k)a}\right)\right]$
$$+B_0\left[g-ik\left(1-e^{i(q+k)a}\right)\right]=0$$

$$\begin{pmatrix}\sim & \sim\\ \sim & \sim\end{pmatrix}\begin{pmatrix}A_0\\ B_0\end{pmatrix}=0 \Rightarrow \det\begin{pmatrix}\sim & \sim\\ \sim & \sim\end{pmatrix}=0$$

$$\Rightarrow \cos(qa)=\cos(ka)+\frac{g}{2k}\sin(ka)$$

Graphical Solution

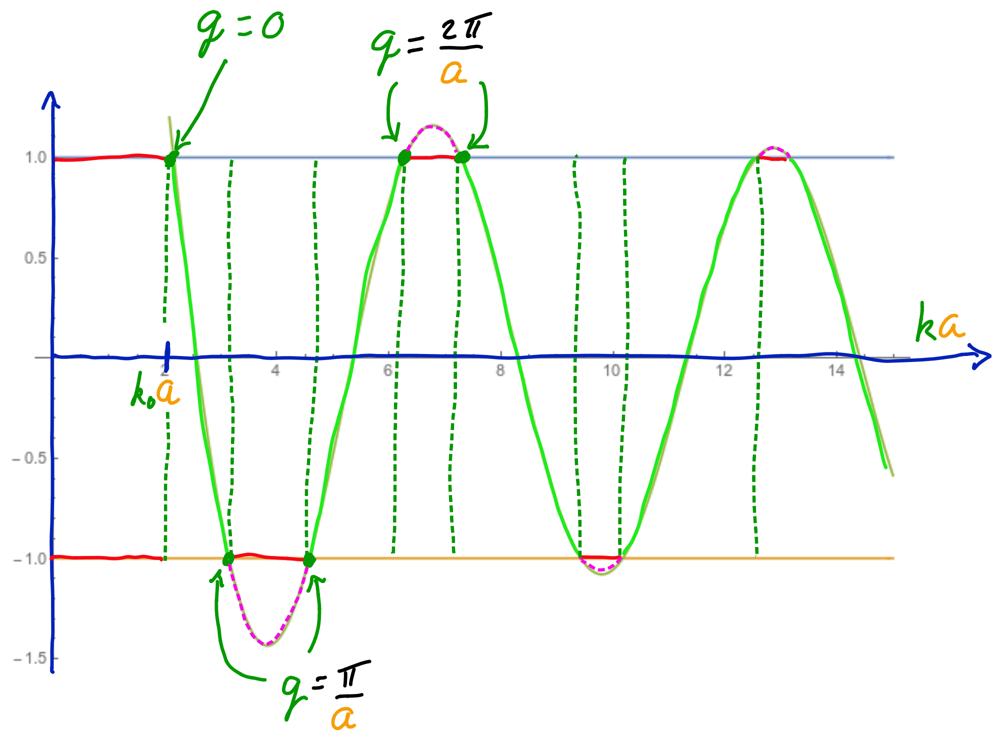
Define $f(ka)\equiv\cos(ka)+\dfrac{ga}{2ka}\sin(ka)$



$|f|>1$ forbidden since

$f(ka)=\cos(qa)\leqslant 1$

$|f|<1$ allowed



Close to band edge: $q \approx 0$ $\quad \cos qa \approx 1 - \frac{1}{2}(qa)^2$

$$f(ka) \approx f(k_0 a) + (k-k_0)\, a\, f'(k_0 a)$$

$$= 1 + (k-k_0)\, a\, f'(k_0 a)$$

$$\Longrightarrow \quad k - k_0 = q^2 a / 2|f'|$$

Recall $E(k) = \frac{\hbar^2 k^2}{2m} = E(k_0) + \frac{\hbar^2(k^2 - k_0^2)}{2m} \approx E_0 + \frac{\hbar^2 k(k-k_0)}{m}$

$$= E_0 + \frac{\hbar^2 k_0}{m} \frac{q^2 a}{2|f'|}$$

Effective mass $\quad \frac{1}{m^*} \equiv \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial q^2} \Longrightarrow \quad \equiv E_0 + \frac{\hbar^2 q^2}{2m^*}$