Spring 2024-25 **EE 207**

HW – 2 Solutions

1. Consider a delta-function potential well $V = -\alpha \cdot \delta(x)$, where $\alpha \in \mathbb{R}$ and $\alpha > 0$.

(a) Integrate the Schrodinger equation to prove that the discontinuity in the first-derivative of the wavefunction at $x = 0$ is given, in this case, by $\Delta\left(\frac{d\psi}{dx}\right) = \frac{-2m\alpha}{\hbar^2}\psi(0)$ (symbols have their usual meanings).

(b) Consider continuum states, i.e. states with $E > 0$. Show that the transmission and reflection probabilities are given by $T = \frac{1}{1+\left(m\alpha^2/2\hbar^2 E\right)}$ and $R = \frac{1}{1+\left(2\hbar^2 E/m\alpha^2\right)}$, respectively.

(c) What are the allowed bound state energies?

(d) What would be the tunneling probability as a function of E for a delta-function barrier $V = +\alpha \cdot \delta(x)$?

(a) The Schrödinger equation is:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \text{ With } V(x) = \alpha\delta(x), \ \alpha \text{ is positive , real.}$$

Let us integrate this in neighborhood of $x = 0$ from $x = -\varepsilon$ to $x = +\varepsilon$.

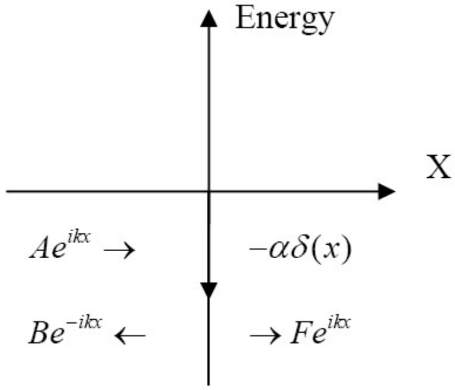
$$\frac{-\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2\psi(x)}{dx^2}dx - \alpha\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)dx = E\int_{-\varepsilon}^{\varepsilon}\psi(x)dx$$

Now as $\varepsilon \to 0$, we have

$$\frac{-\hbar^2}{2m}\left[\Delta\left(\frac{d\psi}{dx}\right)\right]_{x=0} - \alpha\psi(0) = 0$$

$$\left[\Delta\left(\frac{d\psi}{dx}\right)\right]_{x=0} = \frac{-2m\alpha}{\hbar^2}\psi(0)...[1]$$

(b)



For $x > 0^+$ and $x < 0^-$, the Schrödinger equation is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \Rightarrow \frac{d^2\psi(x)}{dx^2} = \frac{-2mE}{\hbar^2} = -k^2\psi$$

The solutions are plane- waves of the form $e^{\pm ikx}$, we assume a plane wave Ae^{ikx} incident from the left and no incident wave from the right. Let the reflected and transmitted wave be Be^{-ikx} and Fe^{ikx} respectively. This is illustrated above.

Now, continuity of $\psi(x)$ at $x = 0 \Rightarrow Ae^{ikx}|_{x=0} + Be^{-ikx}|_{x=o} = Fe^{ikx}|_{x=0}$

$$\Rightarrow A + B = F \ldots[2]$$

And Eq. (1) =>

$$\left[(ik)Fe^{ikx} - \left\{(ik)Ae^{ikx} - (ik)Be^{-ikx}\right\}\right]_{x=0} = \frac{-2m\alpha}{\hbar^2}\left[Fe^{ikx}\right]_{x=0}$$

$$\Rightarrow ik\left[F - A + B\right] = \frac{-2m\alpha}{\hbar^2} \cdot F$$

$$\Rightarrow F - A + F - A = \frac{-2m\alpha}{\hbar^2(ik)} \cdot F \text{ using equation 2}$$

$$\Rightarrow 2(F - A) = \frac{-2m\alpha}{\hbar^2(ik)} \cdot F$$

$$\Rightarrow F\left(1 + \frac{m\alpha}{i\hbar^2 k}\right) = A$$

Transmission amplitude $\Rightarrow t = \dfrac{F}{A} = \dfrac{1}{1 + \dfrac{m\alpha}{i\hbar^2 k}}$

Transmission probability $T = |t|^2 = \dfrac{1}{1+\left(\dfrac{m\alpha}{\hbar^2 k}\right)^2}$

$$T = \frac{1}{1+\dfrac{m^2\alpha^2}{\hbar^2 \cdot \hbar^2 k^2}}$$

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

$$T = \frac{1}{1+\dfrac{m\alpha^2}{2\hbar^2 E}} \ldots [3]$$

Reflection probability $R = 1 - T = \dfrac{1}{1+\left(\dfrac{2\hbar^2 E}{m\alpha^2}\right)}$

(c) We look for bound state in the region $E < 0$.

In this situation $T = \dfrac{1}{1-\dfrac{m\alpha^2}{2\hbar^2 |E|}}$

For a bound state $T \to \infty$. This implies that

$$1-\frac{m\alpha^2}{2\hbar^2 |E|} = 0 \Rightarrow |E| = \frac{m\alpha^2}{2\hbar^2}$$

$$\Rightarrow E = -\frac{m\alpha^2}{2\hbar^2}$$

This is the energy eigenvalue for the only bound state the delta function well supports.

Alternatively, the bound state can be found as we did in class, which is as follows.

The wavefunction is:

$$\psi(x) = \begin{matrix} C_+ e^{-\kappa x}, \ x > 0 \\ C_- e^{+\kappa x}, \ x < 0 \end{matrix} \ldots [4]$$

where $\kappa = \sqrt{\dfrac{2m(-E)}{\hbar^2}}$.

Continuity of the wavefunction at the origin implies: $C_+ = C_- = \psi(0)$

The discontinuity in $d\psi/dx$ at the origin given in Eq. [1] may now be written as:

$$\left[\Delta\left(\frac{d\psi}{dx}\right)\right]_{x=0} = -\kappa\psi(0) - \left(\kappa\psi(0)\right) = -2\kappa\psi(0) = \frac{-2m\alpha}{\hbar^2}\psi(0)$$

$$\Rightarrow \kappa = \frac{m\alpha}{\hbar^2}$$

$$\Rightarrow \frac{2m(-E)}{\hbar^2} = \frac{m^2\alpha^2}{\hbar^4}$$

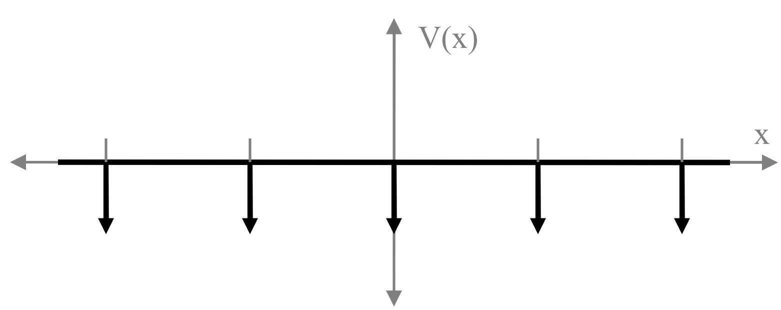
$$\Rightarrow E = -\frac{m\alpha^2}{2\hbar^2}$$

(d) If $V = \alpha\delta(x)$ We only need to flip the sign of α in equation (3). This gives us, for the delta function barrier, a tunneling probability.

$$T = \frac{1}{1 + \frac{m\alpha^2}{2\hbar^2 E}}$$

which is the same as that for the well.

2. Let us model the periodic electric potential in a (one-dimensional) crystalline solid by the "Dirac-comb" potential: $V(x) = -\alpha\sum_{j=0}^{N-1}\delta(x - ja)$ illustrated below, where N is the number of atoms. Use the Bloch theorem and the known solution to the single Dirac potential well (from problem #1 above) to find out the allowed energies. You should also find some forbidden 'gaps' in the spectrum, and thus we obtain bands. How many allowed states do you have in each band? Consider the filling of these allowed states by electrons contributed by the atoms (note: remember the Pauli Exclusion Principle for electrons). Comment on the situation when each of the N atoms contributes 1 free electron, versus when they contribute 2 each.



In the region $(0,a)$, we have

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2}=-k^2\psi,$$

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

The general solution is

$$\psi(x)=A\sin kx+B\cos kx,\ \text{for}\ x\in(0,a)$$

Using Bloch's Theorem $\left\{\psi(x+a)=e^{iKa}\psi(x)\right\}$

$$\psi(x)=e^{-iKa}\left[A\sin k(x+a)+B\cos k(x+a)\right]\ \text{for}\ x\in(-a,0)$$

Now, we know (mid-sem problem) that

$$\psi(0^+)=\psi(0^-)\ \text{and}\ \left[\Delta\left(\frac{d\psi}{dx}\right)\right]_{x=0}=\frac{-2m\alpha}{\hbar^2}$$

The continuity of $\psi(x)$ at $x=0$ implies:

$$B=e^{-iKa}\left[A\sin(ka)+B\cos(ka)\right]\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

The discontinuity of $\psi'(x)$ at $x=0$ implies

$$kA-e^{-iKa}k\left[A\cos(ka)-B\sin(ka)\right]=\frac{-2m\alpha}{\hbar^2}B\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

$$(1)\Rightarrow A\sin(ka)=\left[e^{iKa}-\cos(ka)\right]B$$

Using this in (2) and cancelling kB :

$$\left(e^{iKa}-\cos(ka)\right)\left(1-e^{-iKa}\cos(ka)\right)+e^{-iKa}\sin^2(ka)=\frac{-2m\alpha}{\hbar^2k}\sin(ka)$$

$$\Rightarrow \cos(Ka)=\cos(ka)-\frac{m\alpha}{\hbar^2k}\sin(ka)\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

Let $z=ka$ and $\beta=\frac{m\alpha a}{\hbar^2}$

$$(3)\Rightarrow f(z)=\cos z-\beta\frac{\sin z}{z}=\cos(Ka)\ldots\ldots\ldots\ldots(4)$$

Note that solution exist if $-1 \le f(z) \le 1$. This gives rise to allowed energy bands and forbidden gaps as shown in Fig.4.

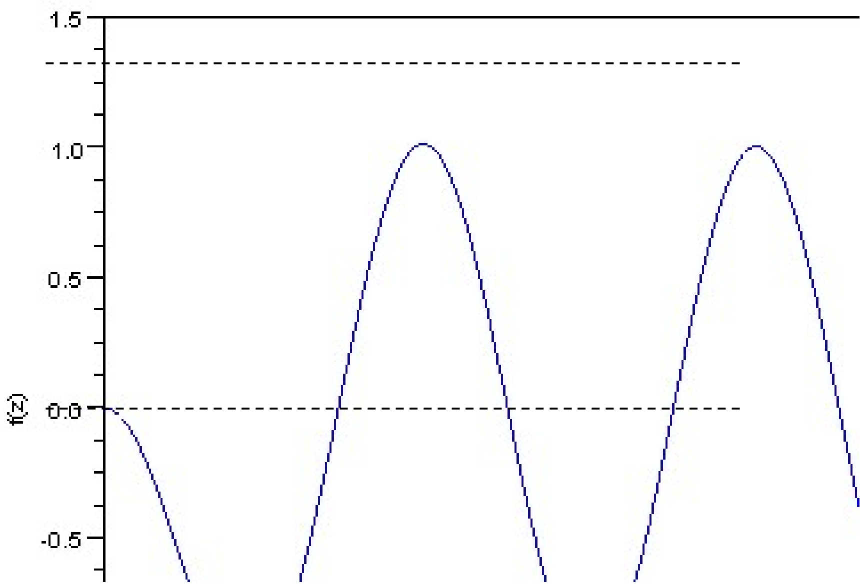


Fig. 4. Allowed bands where the $RHS \in [-1,1]$ and forbidden gaps.

Now imposing the periodic boundary condition, $\psi(x+Na)=\psi(x)$, where $N \sim 10^{23}$ is the# of atoms, we get from Bloch's theorem:

$$e^{iKNa}\psi(x)=\psi(x)$$

$$\Rightarrow e^{iKNa}=1 \Rightarrow KNa = 2\pi n, n = 0, \pm 1, \pm 2, \ldots\ldots\ldots\ldots$$

$\Rightarrow K = \dfrac{2\pi}{Na}\cdot n,\ \ n \in z$ are the allowed K values subject to equation (4).

In every band, we have N allowed values of K for $n=0$ to $n=N-1$. This is seen by drawing N horizontal lines at the values of $\cos(Ka)=\cos\left(\dfrac{2\pi n}{N}\right)$ (note that the lines for $\pm K$ coincide). This is illustrated in the attached Scilab program named 'Bands'.

If we have free $2N$ electrons per atom the first band will be completely filled – remember we can have 2 electrons in every k-state- and we get an insulator. On the other hand, for 1 free electron per atom, the first-band is only half-filled and we have a metal.