Lecture 5 Particle Waves in One Dimension

SCPY152, Second Semester 2021-22

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Topics

Example of particle wave functions (stationary) derived from Schrodinger's equation (SE). Different problem (equation) comes from different potential term $U(x)$, we start with some simple systems in one dimension, i.e.,

1. Free particle
2. Potential step
3. Potential barrier

To be easy for looking for solution, we may rewrite SE in suitable form for getting its solution as

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} + U(x)\varphi(x) = E\varphi(x)$$

$$\mapsto \varphi''(x) + \frac{2m}{\hbar^2}\left(E - U(x)\right)\varphi(x) = 0,\ \varphi'' = \frac{d^2\varphi}{dx^2} \tag{1}$$

Free Particle

In case of free particle, the potential energy is constant and set to be zero $U = 0$ for convenient. Its SE is

$$\begin{aligned} \varphi'' + k^2\varphi = 0 \mapsto \varphi(x) &= C_1 e^{+ikx} + C_2 e^{-ikx} \\ &\equiv \varphi_1(x) + \varphi_2(x) \end{aligned} \tag{2}$$

Its physical interpretations are

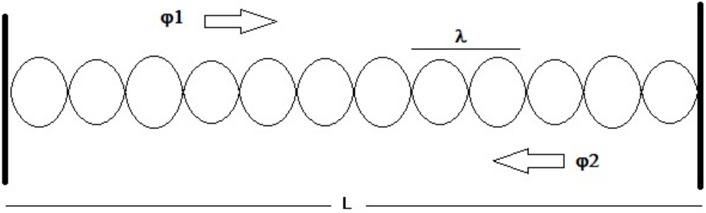
$$\varphi_1(x) - \text{the right mover} \qquad \varphi_2(x) - \text{the left mover}$$

Assign with quantum statistical meaning, normalization in a large box of size L is

$$1 = \int_0^L |\varphi_{1/2}(x)|^2 dx = |C_{1/2}|^2 \int_0^L dx = |C_{1/2}|^2 L \mapsto C_{1/2} = \frac{1}{\sqrt{L}} \tag{3}$$

$$\varphi_{1/2}(x) = \frac{1}{\sqrt{L}} e^{\pm ikx} \tag{4}$$

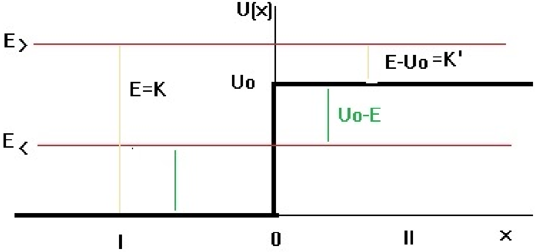
With $k = 2\pi/\lambda$, we observe these free particle waves in the form



Potential Step

In case of particle of energy E travels between two regions with different potential energy

$$U(x) = \begin{cases} 0, & x < 0 \\ U_0, & x > 0 \end{cases}$$



We separate x in to two regions, i.e., region I for $x < 0$ and region II for $x > 0$.

Write SE in both regions and their solutions:

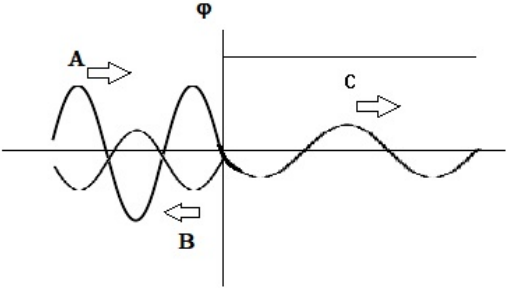
- In case of $E > U_0$:

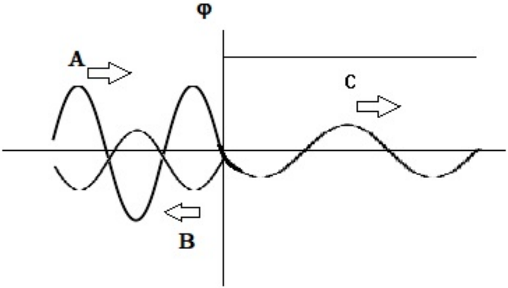
$$I: \qquad \varphi_I'' + k^2\varphi_I = 0 \mapsto \ \varphi_I(x) = Ae^{ikx} + Be^{-ikx} \tag{5}$$
$$II: \qquad \varphi_{II}'' + k'^2\varphi_{II} = 0 \mapsto \ \varphi_{II}(x) = Ce^{ik'x} + De^{-ik'x} \tag{6}$$

  where $k^2 = 2mE/\hbar^2, \ k'^2 = 2m(E - U_0)/\hbar^2$.

  - A is amplitude of particle wave come in from the left
  - B is amplitude of particle wave reflects from potential step back to the left
  - C is amplitude of particle wave pass though the potential step to the right
  - D is amplitude of particle wave come in from the right, actually we do not this wave so we will set $D = 0$ Then we have particle wave in the form

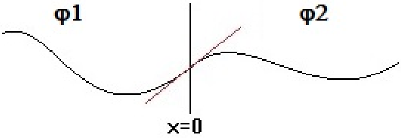
$$\varphi_I(x) = Ae^{ikx} + Be^{-ikx}, \ \varphi_{II}(x) = Ce^{ik'x}$$


φ
A
C
B



Connect the two waves *continuously* at the boundary $x = 0$, with conditions

$$\varphi_I(0) = \varphi_{II}(0), \quad \varphi_I'(0) = \varphi_{ii}'(0)$$



From above we will have

$$A + B = C \qquad ik(A - B) = ik'C \mapsto A - B = \frac{k'}{k}C \tag{7}$$

$$\mapsto \frac{C}{A} = \frac{2k}{k + k'}, \ \frac{B}{A} = \frac{k - k'}{k + k'} \tag{8}$$

Now we can assign the potential step tunneling coefficient T and reflection coefficient R of the particle wave as

$$T = \left|\frac{C}{A}\right|^2 = \frac{4k^2}{k + k'}^{2}, \ R = \left|\frac{B}{A}\right|^2 = \frac{(k - k')^2}{(k + k')^2} \tag{9}$$

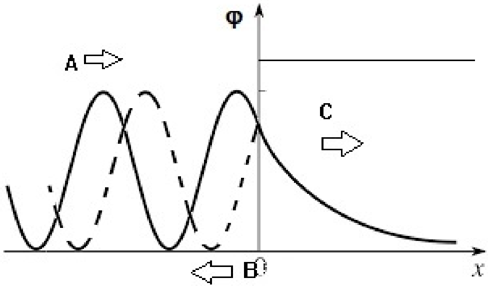
$$\mapsto T + R = 1 \tag{10}$$

- In case of $E < U_0$: SE and their solutions in both regions become

$$I: \quad \varphi_I'' + k^2\varphi_I = 0 \mapsto \varphi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (11)$$
$$II: \quad \varphi_{II}'' - \kappa^2\varphi_{II} = 0 \mapsto \varphi_{II}(x) = Ce^{-\kappa x} + De^{\kappa x} \quad (12)$$

where $\kappa^2 = 2m(U_0 - E)/\hbar^2$. Now A and B get the same meanings as before but for C and D they are

  - C is the particle eave attenuate into the step on the right
  - D is particle wave growing into the the potential step on the right, which is not really happen so we have to set $D = 0$



Connection of the two particle waves at $x = 0$

$$A + B = C \qquad ik(A - B) = \kappa C \mapsto A - B = \frac{\kappa}{ik} C \tag{13}$$

$$\frac{C}{A} = \frac{2ik}{ik + \kappa}, \; \frac{B}{A} = \frac{ik - \kappa}{ik + \kappa} \mapsto R = 1 \tag{14}$$

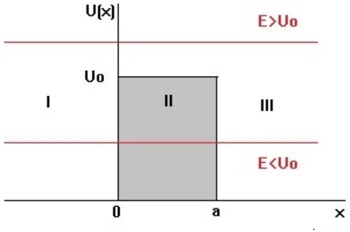
Actually particle wave totally reflects from the potential step back to the left.
Penetration distance d into the potential step is determined to be $1/e$ reduction as

$$d = \frac{1}{\kappa}$$

Potential Barrier

Let there be a potential barrier $U(x)$ as

$$U(x) = \begin{cases} 0, & x < 0 \\ U_0, & 0 < x < a \\ 0, & x > a \end{cases}$$



In this problem we have three regions of x, write SE ans their solutions in all regions

- In case of $E > U_0$, with $k^2 = 2mE/\hbar^2, k'^2 = 2m(E - U_0)/\hbar^2$,

$$I: \quad \varphi_I'' + k^2\varphi_I = 0 \mapsto \varphi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (15)$$
$$II: \quad \varphi_{II}'' + k'^2\varphi_{II} = 0 \mapsto \varphi_{II}(x) = Ce^{ik'x} + De^{-ik'x} \quad (16)$$
$$III: \quad \varphi_{III}'' + k^2\varphi_{III} = 0 \mapsto \varphi_{III}(x) = Fe^{ikx} + Ge^{-ikx} \quad (17)$$

As before

- A is amplitude of particle wave incoming wave from the left
- B is amplitude of particle wave reflection wave back to the left
- C, D are amplitude of particle waves reflect back and forth inside the barrier
- F is amplitude of particle wave that pass though the barrier
- G is amplitude of particle wave coming from the right, since we do not have this kind of wave so we will set $G = 0$

Connect φ_I with φ_{II} at $x = 0$, and φ_{II} with φ_{III} at $x = a$.

$$A + B = C + D \tag{18}$$

$$ik(A - B) = ik'(C - D) \tag{19}$$

$$C^{ik'a} + De^{-ik'a} = Fe^{ika} \tag{20}$$

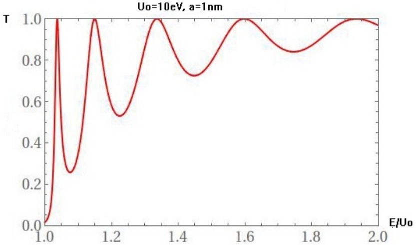
$$ik'(Ce^{ik'a} - De^{-ik'a}) = ikFe^{ika} \tag{21}$$

Solve these equations for A, B, F, in order to determine $R = |B/A|^2$ - reflection coefficient and $T = |F/A|^2$ - tunneling coefficient. We do have

$$\left|\frac{B}{A}\right| = \frac{(k^2 - k'^2)\sin(k'a)}{(k^2 + k'^2)\sin(k'a) - 2kk'\cos(k'a)} \tag{22}$$

$$\left|\frac{F}{A}\right| = \frac{2kk'}{2kk'\cos(k'a) - (k^2 + k'^2)\sin(k'a)} \tag{23}$$

Note that when $k'a = 2n\pi$, $n = 1, 2, ...$, the particle wave will totally 100% pass through the barrier without any reflection. This is called *resonance tunneling*. This is used to detect the size a of the barrier, by measuring 100% tunneling over the barrier .



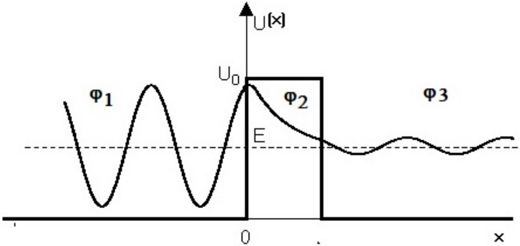
Derivation of (22,23) is a challenge only for smart students!!

- In case of $E < U_0$, we will have SE in all regions in the form

$$
\begin{aligned}
I: &\quad \varphi_I'' + k^2\varphi_I = 0 \mapsto \varphi_I(x) = Ae^{ikx} + Be^{-ikx} && (24)\\
II: &\quad \varphi_{II}'' - \kappa^2\varphi_{II} = 0 \mapsto \varphi_{II}(x) = Ce^{-\kappa x} + De^{\kappa x} && (25)\\
III: &\quad \varphi_{III}'' + k^2\varphi_{III} = 0 \mapsto \varphi_{III}(x) = Fe^{ikx} && (26)
\end{aligned}
$$

Now we have attenuation waves inside the barrier with amplitudes D and D with coefficient

$$\kappa^2 = \frac{2m(U_0 - E)}{\hbar^2}$$



As before, we have to connect these waves at $x = 0$ and $x = a$, and solving the connection equations for A, B and F for calculating the coefficients $R = |B/A|^2$ and $T = |F/A|^2$.
Anyway we can use our previous result by a bit changing of $k' = -i\kappa$ and use the fact that $\sin(k'a) = i\sinh(\kappa a)$ and $\cos(k'a) = \cosh(\kappa a)$. From (23) we do have

$$\left|\frac{F}{A}\right| = \frac{2k\kappa}{2k\kappa\cosh(\kappa a) + (k^2 - \kappa^2)\sinh(\kappa a)} \tag{27}$$

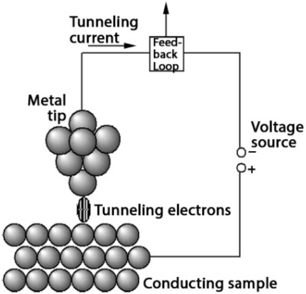
In the limit of $\kappa a \ll 1$ we will have the tunneling coefficient (probability) in the form

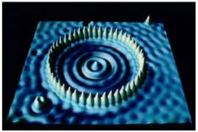
$$T \simeq e^{-2\kappa a} \tag{28}$$

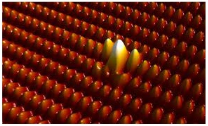
Rewrite this expression for more applicable calculation in the form

$$T \simeq \exp\left\{-2\int_0^a \kappa(x)dx\right\}, \;\; \kappa(x) = \sqrt{\frac{2m}{\hbar^2}(U(x) - E)} \tag{29}$$

Scanning probe tunneling electron microscope (STM)







Gamow theory of alpha emission from the atomic nucleus