PH 107 :Quantum Physics and Applications

Step potential

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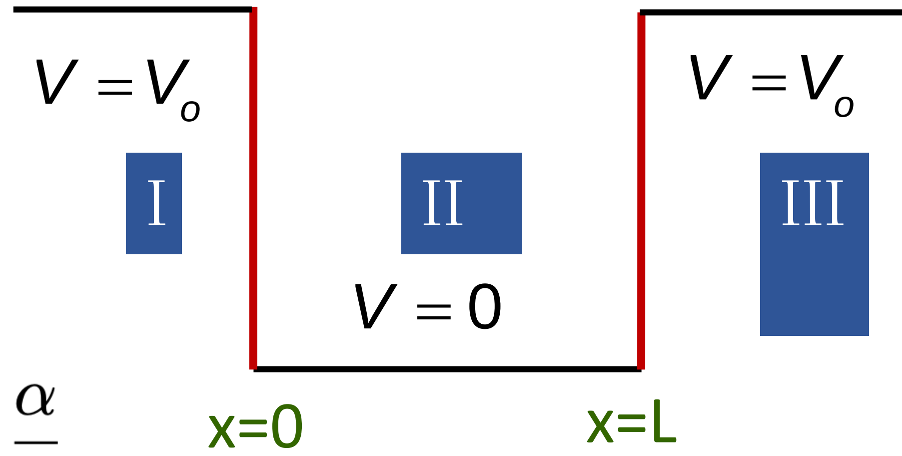
Recap (Finite Potential Well)



$$V(x) = 0 \quad \text{for } 0 < x < L$$
$$= V_o \quad \text{for x} < 0 \text{ or } x > L$$

$$\tan\left(\frac{kL}{2}\right) = \frac{\alpha}{k} \qquad -\cot\left(\frac{kL}{2}\right) = \frac{\alpha}{k}$$

$$tan\left(\frac{kL}{2}\right) = \sqrt{\left(\frac{k_o L/2}{kL/2}\right)^2 - 1}$$

$$\text{and } -cot\left(\frac{kL}{2}\right) = \sqrt{\left(\frac{k_o L/2}{kL/2}\right)^2 - 1}$$

Using $\dfrac{2m}{\hbar^2}(V_0 - E) = \alpha^2$;

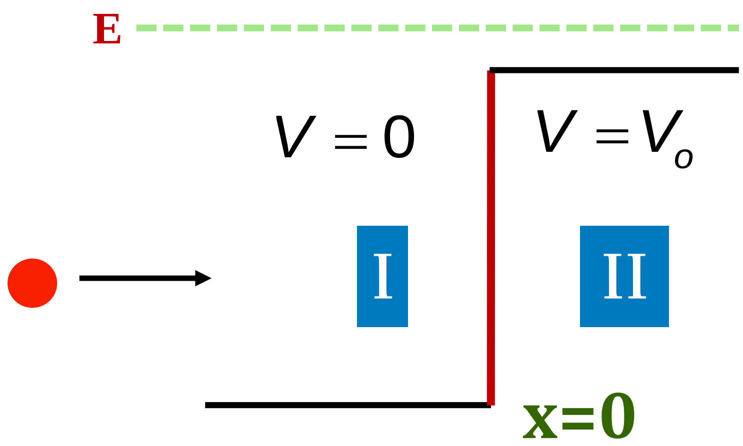
$$\frac{2mE}{\hbar^2} = k^2$$

and $k_0 = \sqrt{\dfrac{2mV_0}{\hbar^2}}$

Graphical intersection of LHS and RHS is the estimate of the allowed energy states.

Step potential

$$V(x) = 0 \qquad \forall x \leq 0$$
$$\qquad = V_0 \qquad \forall\, x > 0$$



Consider, E > V_0

Classically, there will be total transmission of all particles and particle will have kinetic energy E - V_0. This is a simple *scattering* problem in 1-D.

Quantum mechanically, the dynamics is regulated by SE.

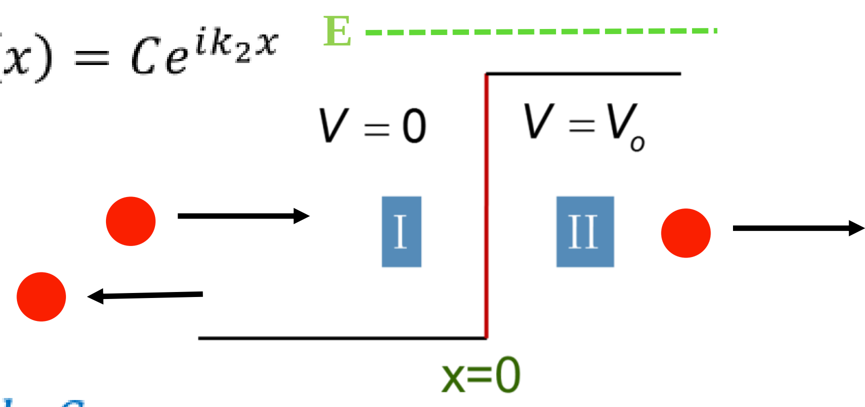
$$\varphi_1(x) = Ae^{i\,k_1 x} + Be^{-i\,k_1 x} \text{ ,where } k_1^2 = \frac{2mE}{\hbar^2}, \text{ X} < 0$$

$$\varphi_{II}(x) = Ce^{i\,k_2 x} + De^{-i\,k_2 x} \text{ ,where } k_2^2 = \frac{2m(E - V_o)}{\hbar^2}, \text{ X} > 0$$

1. **Since there is no incidence from the right side, in**

$$\varphi_{II}(x) = Ce^{ik_2x} + De^{-ik_2x} \Rightarrow D = 0$$

$$\Rightarrow \varphi_{II}(x) = Ce^{ik_2x}$$



2. **Boundary conditions**

(a) $\varphi_I(0) = \varphi_{II}(0) \Longrightarrow A + B = C$

(b) $\varphi_I'(0) = \varphi_{II}'(0) \Longrightarrow ik_1(A - B) = ik_2C$

Add

$$\Longrightarrow A = \frac{C}{2}\left(1 + \frac{k_2}{k_1}\right)$$

Divide

$$\Longrightarrow \frac{C}{A} = \frac{2k_1}{k_1 + k_2}$$

Subtract

$$\Longrightarrow B = \frac{C}{2}\left(1 - \frac{k_2}{k_1}\right)$$

Divide

$$\Longrightarrow \frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$

The wave functions; $\varphi_I(x) = A\left(e^{ik_1x} + \left(\frac{k_1-k_2}{k_1+k_2}\right)e^{-ik_1x}\right)$, X < 0

in terms of A $\varphi_{II}(x) = A\left(\frac{2k_1}{k_1+k_2}\right)e^{ik_2x}$, X < 0

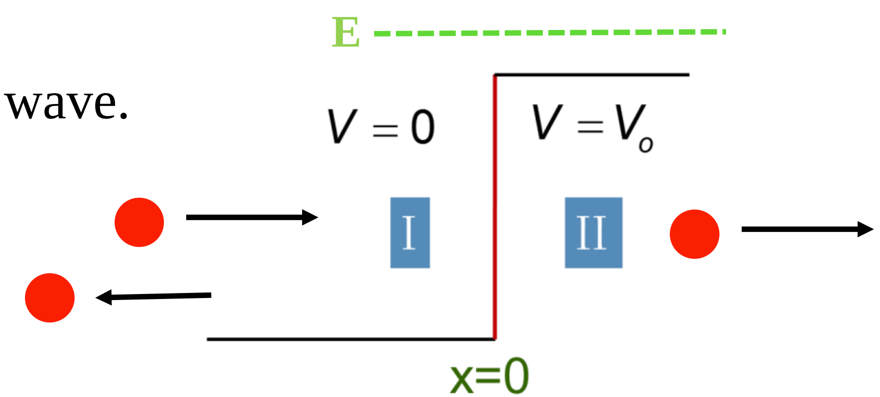
- This implies that the probability of the particle being **reflected** is non-zero. However classically this is forbidden.

- This effect is attributed to wave like behavior of particles.

Ae^{ik_1x} represents the incident wave

$A\left(\frac{k_1-k_2}{k_1+k_2}\right)e^{-ik_1x}$ represents the reflected wave

$A\left(\frac{2k_1}{k_1+k_2}\right)e^{ik_2x}$ represents the transmitted wave.



Probability Density, E > V_0

Ae^{ik_1x} represents the incident wave

$A\left(\frac{k_1-k_2}{k_1+k_2}\right)e^{-ik_1x}$ represents the reflected wave

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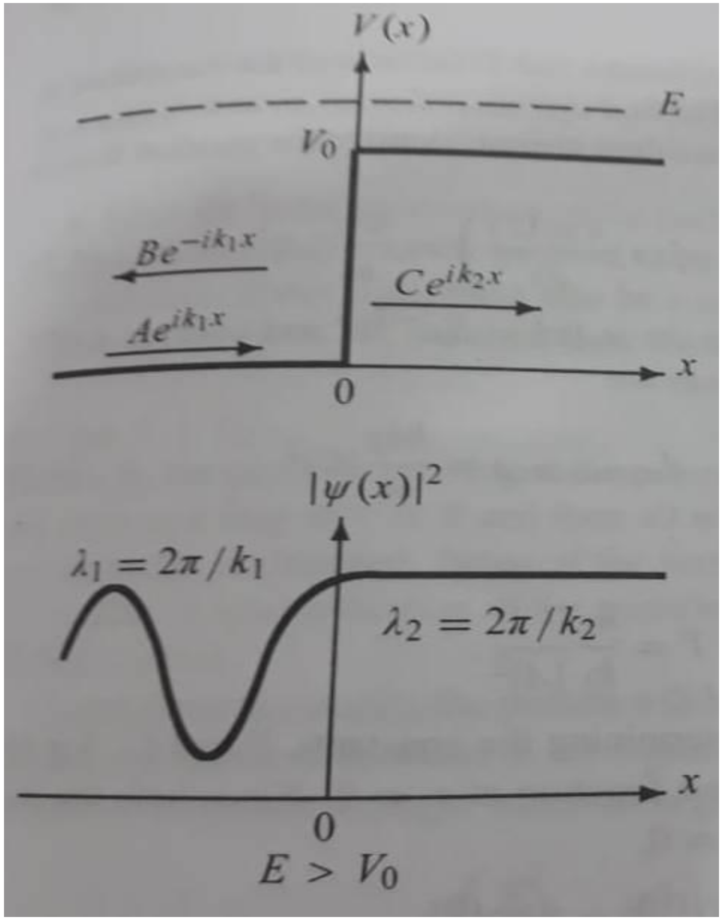
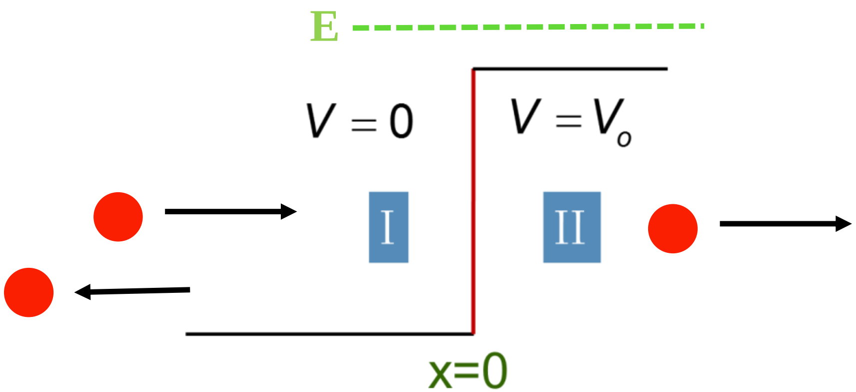




Case E = Vo

$$\varphi_1(x) = Ae^{i\,k_1 x} + Be^{-i\,k_1 x}\text{,where } k_1^2 = \frac{2mE}{\hbar^2} \quad , \text{X} < 0$$

$$\varphi_{II}(x) = Ce^{i\,k_2 x} \qquad \text{,where } k_2^2 = \frac{2m(E - V_o)}{\hbar^2} \text{ , X} > 0$$

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$

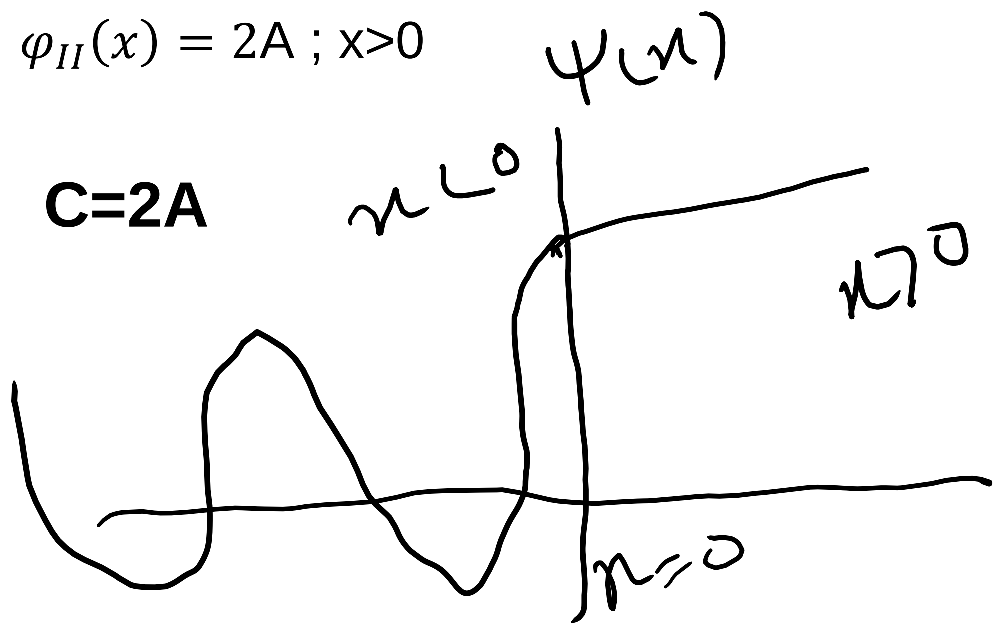
B=A

$$\varphi_1(x) = 2ACos\,k_1 x \quad , \text{X} < 0$$

$\varphi_{II}(x) =$ 2A ; x>0

$$\frac{C}{A} = \frac{2k_1}{k_1 + k_2}$$

C=2A



Probability current density

$$J(x,t) = \frac{\hbar}{2im}\left[\psi*(x,t)\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial\psi*(x,t)}{\partial x}\right]$$

J (x,t) is the current associated with charge density ρ

Derivation provided in lecture notes

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$$

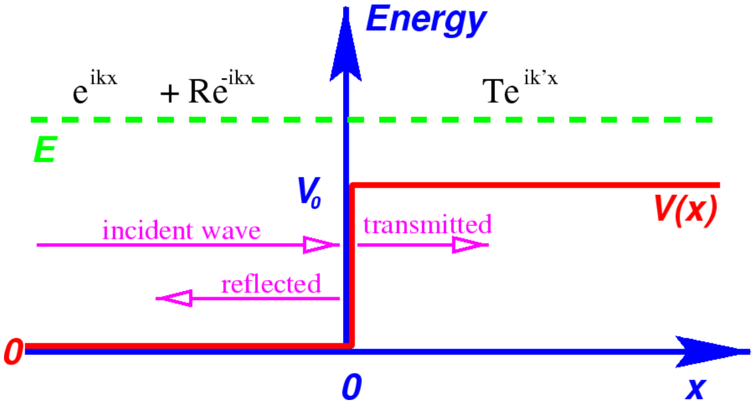
Change in charge is associated with current escaping/entering the volume.

Charge density in electromagnetism is equivalent to probability density in Quantum Mechanics.

Probability Current density

The current density/flux is defined as :

$$J = \frac{\hbar}{2im}\left[\psi*(x,t)\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial\psi*(x,t)}{\partial x}\right]$$



$$\varphi_1(x) = Ae^{i\,k_1 x} + Be^{-i\,k_1 x}, \text{where } k_1^2 = \frac{2mE}{\hbar^2} \quad , X < 0$$

$$\varphi_{II}(x) = Ce^{i\,k_2 x} + De^{-i\,k_2 x}, \text{where } k_2^2 = \frac{2m(E-V_o)}{\hbar^2}, X > 0$$

$$j_{incident} = \frac{\hbar\,k_1}{m}|A|^2 \qquad j_{reflected} = \frac{-\hbar\,k_1}{m}|B|^2$$

$$j_{transmitted} = \frac{\hbar\,k_2}{m}|C|^2$$

Probability Current density

The rate at which the incident particles approach the barrier is $(\hbar k_1/m)|A|^2$.

The rate at which they are reflected is $(\hbar k_1/m)|B|^2$

and the rate at which they move forward is $(\hbar k_2/m)|C|^2$.

The factor of $\frac{k_2}{k_1}$ in T due to different rate at which the incident and transmitted particles move in region I and II.

$$j_{x<0} = \frac{\hbar\, k_1}{m}\left[|A|^2 - |B|^2\right] \qquad j_{x>0} = \frac{\hbar\, k_2}{m}|C|^2$$

Conversation of Probability Current

$$j_{x<0} = \frac{\hbar k_1}{m}[|A|^2 - |B|^2] \qquad j_{x>0} = \frac{\hbar k_2}{m}|C|^2$$

These two currents density should be same.

$$\frac{\hbar k_1}{m}[1 - \frac{|B|^2}{|A|^2}]\,|A|^2 = \frac{\hbar k_1}{m}[1 - \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2]\,|A|^2$$

$$= \frac{\hbar k_1}{m}[\frac{4k_1k_2}{(k_1+k_2)^2}]\,|A|^2$$

$$= \frac{\hbar k_2}{m}[\frac{4k_1^2}{(k_1+k_2)^2}]\,|A|^2$$

$$= \frac{\hbar k_2}{m}\,|C|^2$$

Conservation of probability current holds

Transmission and Reflection coefficients

Reflection coefficient,

$$R = \left|\frac{reflected\ current\ density}{incident\ current\ density}\right| = \left|\frac{J_{reflected}}{J_{incident}}\right|$$

Transmission coefficient,

$$T = \left|\frac{transmitted\ current\ density}{incident\ current\ density}\right| = \left|\frac{J_{transmitted}}{J_{incident}}\right|$$

To estimate the reflection and transmission coefficient, we should the wave function in the appropriate region.

$$\varphi_I(x) = A\left(e^{ik_1x} + \left(\frac{k_1 - k_2}{k_1 + k_2}\right)e^{-ik_1x}\right) \quad \varphi_{II}(x) = A\left(\frac{2k_1}{k_1 + k_2}\right)e^{ik_2x}$$

$$j_{incident} = \frac{\hbar\, k_1}{m}|A|^2 \quad j_{reflected} = \frac{-\hbar\, k_1}{m}|B|^2 \quad j_{transmitted} = \frac{\hbar\, k_2}{m}|C|^2$$

Reflection coefficient, $R = \left|\frac{B}{A}\right|^2 = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$

Transmission coefficient, $T = \frac{k_2}{k_1}\left|\frac{C}{A}\right|^2 = \frac{4k_1k_2}{(k_1 + k_2)^2}$

- In contrast to classical mechanics, which states that none of the particles gets reflected, quantum mechanical reflection coefficient , $R \neq 0$.
- There are particles that get reflected inspite of $E > V_o$. This effect must be attributed to the ***wavelike behavior*** of the particles.
- The sum of Reflection and Transmission coefficient,

$$R + T = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 + \frac{4k_1k_2}{(k_1 + k_2)^2} = 1$$

Transmission and Reflection coefficients, E > V_0

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 = \left(\frac{1-\kappa}{1+\kappa}\right)^2$$

$$T = \frac{4k_1k_2}{(k_1+k_2)^2} = \frac{4\kappa}{(1+\kappa)^2}$$

where $\kappa = \frac{k_2}{k_1} = \sqrt{\mathbf{1} - \frac{\boldsymbol{V_o}}{\boldsymbol{E}}}$

- For small value of E, T decreases.
- For E = $\boldsymbol{V_0}$, T = 0 and R =1.
- For E >>> $\boldsymbol{V_0}$, κ ~1, hence R = 0 and T =1.
- Particles with very high energies, the potential step is so weak that it produces no noticeable effect on their motion.

Continuity equations

Schrodinger Equation for $\psi(x, t)$

$$i\hbar \frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \qquad (1)$$

Schrodinger Equation for $\psi * (x, t)$

$$i\hbar \frac{\partial\psi*(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi*(x,t)}{\partial x^2} + V(x)\psi * (x,t) \qquad (2)$$

Multiply 1 by $\psi * (x, t)$ and 2 by $\psi(x, t)$

$$i\hbar\psi * (x,t)\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\psi * (x,t)\frac{\partial^2\psi(x,t)}{\partial x^2} + \psi * (x,t)V(x)\psi(x,t) \qquad (3)$$

$$i\hbar\psi(x,t)\frac{\partial\psi*(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\psi(x,t)\frac{\partial^2\psi*(x,t)}{\partial x^2} + \psi(x,t)V(x)\psi*(x,t) \quad (4)$$

Subtract eq 3 from eq 4

$$\boxed{i\hbar\left[\psi*(x,t)\frac{\partial\psi(x,t)}{\partial t} + \psi(x,t)\frac{\partial\psi*(x,t)}{\partial t}\right] = -\frac{\hbar^2}{2m}\left[\psi*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2} - \psi(x,t)\frac{\partial^2\psi*(x,t)}{\partial x^2}\right]} \quad (5)$$

Since

$$\frac{\partial\psi*(x,t)\psi(x,t)}{\partial t} = \psi*(x,t)\frac{\partial\psi(x,t)}{\partial t} + \frac{\partial\psi*(x,t)}{\partial t}\psi(x,t)$$

$$\frac{\partial}{\partial x}\left\{\psi *(x,t)\frac{\partial\psi(x,t)}{\partial x}-\psi(x,t)\frac{\partial\psi*(x,t)}{\partial x}\right\}$$

$$=\frac{\partial\psi*(x,t)}{\partial x}\frac{\partial\psi(x,t)}{\partial x}+\psi *(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2}-\frac{\partial\psi(x,t)}{\partial x}\frac{\partial\psi*(x,t)}{\partial x}-\psi(x,t)\frac{\partial^2\psi*(x,t)}{\partial x^2}$$

$$=\psi *(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2}-\psi(x,t)\frac{\partial^2\psi*(x,t)}{\partial x^2}$$

$$\boxed{\frac{\partial}{\partial x}\left\{\psi *(x,t)\frac{\partial\psi(x,t)}{\partial x}-\psi(x,t)\frac{\partial\psi*(x,t)}{\partial x}\right\}=\psi *(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2}-\psi(x,t)\frac{\partial^2\psi*(x,t)}{\partial x^2}}$$

(6)

From eqn 5

$$i\hbar\left[\psi*(x,t)\frac{\partial\psi(x,t)}{\partial t}+\psi(x,t)\frac{\partial\psi*(x,t)}{\partial t}\right]=-\frac{\hbar^2}{2m}\left[\psi*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2}-\psi(x,t)\frac{\partial^2\psi*(x,t)}{\partial x^2}\right]$$

$$\Rightarrow$$

$$i\hbar\left[\frac{\partial\psi(x,t)\psi*(x,t)}{\partial t}\right]=-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left[\psi*(x,t)\frac{\partial\psi(x,t)}{\partial x}-\psi(x,t)\frac{\partial\psi*(x,t)}{\partial x}\right]$$

$$\Rightarrow\quad i\hbar\left[\frac{\partial\psi(x,t)\psi*(x,t)}{\partial t}\right]+\frac{\hbar^2}{2im}\frac{\partial}{\partial x}\left[\psi*(x,t)\frac{\partial\psi(x,t)}{\partial x}-\psi(x,t)\frac{\partial\psi*(x,t)}{\partial x}\right]=0$$

$\rho=\psi(x,t)\psi*(x,t)$ = probability

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$$

J (x,t) is the current associated with charge density ρ

$$\boxed{J = \frac{\hbar}{2im}\left[\psi * (x,t)\frac{\partial \psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial \psi * (x,t)}{\partial x}\right]}$$