

Introduction to Quantum Mechanics

INEL 5209 - Solid State Devices - Spring 2012

Manuel Toledo

January 23, 2012

Outline

- 1 Review
 - Time dependent Schrödinger equation
 - Momentum operator
 - Time-independent form of SE
 - Free Particle
- 2 Electron Meeting a Potential Barrier
- 3 Tunneling
- 4 The Quantum Well

Schrödinger equation

Time dependent Schrödinger equation (SE):

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + U(x,y,z)\Psi$$



Momentum operator

$$\frac{\hbar}{i} \frac{\partial}{\partial r}$$

r can be x , y or z .

Expectation value of the momentum in the x direction:

$$\langle p_x \rangle = \int_V \Psi^* \frac{\hbar}{i} \frac{\partial \Psi}{\partial x} dV$$

Energy operator:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

Time-independent form of SE

$$\nabla^2\psi + \frac{2m}{\hbar^2} (E - U(x, y, z)) \psi = 0$$

Free Particle

Consider a particle of mass m in a 1D space that

- is isolated - infinitely far from other particles
- has total particle energy is E
- experiences no forces ($\mathbf{F} = \nabla U = 0$)
- and thus has constant potential energy (chosen to be 0).

From the POV of QM to characterize the particle one must solve the time-independent Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad (1)$$

For free particle,

$$\Psi(x, t) = Ae^{i(kx - \frac{E}{\hbar}t)} + Be^{-i(kx + \frac{E}{\hbar}t)}$$

- The free particle wave-function is similar to a traveling wave.

For free particle,

$$\Psi(x, t) = Ae^{i(kx - \frac{E}{\hbar}t)} + Be^{-i(kx + \frac{E}{\hbar}t)}$$

- The free particle wave-function is similar to a traveling wave.
- If the particle moves in the x direction, $B = 0$. If it moves in the $-x$ direction, $A = 0$.
- Since, for a particle moving in the $+x$ direction,

$$\psi^* \psi = A^* A = \text{constant}$$

for all values of x , one has equal probability of finding the particle anywhere.

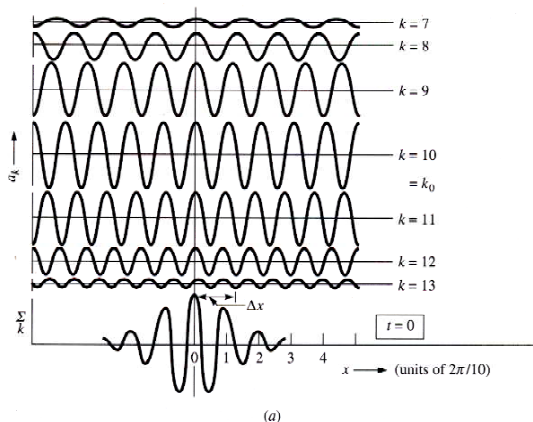
Momentum

The particle's momentum is

$$\begin{aligned}\langle p_x \rangle &= \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i} \frac{d\psi}{dx} dx \\ &= \hbar k \int_{-\infty}^{\infty} \psi^* \psi dx \\ &= \hbar k = \frac{h}{\lambda} = \sqrt{2mE}\end{aligned}$$

in agreement with classical mechanics.

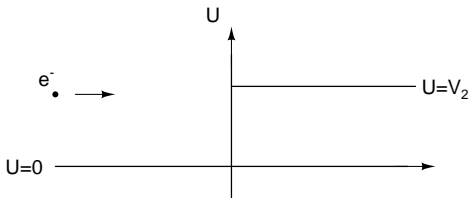
Wave-packet



Example illustrating wave-function superposition. (Taken from Craig Casey, 1999).

Potential barrier

Consider a 1D potential with the shape shown below.



An electron approaching a potential barrier.

We must now solve two equations. For $x \leq 0$ the electron is free ($U = 0$), and the solution is the one found for a free particle:

$$\psi = Ae^{ikx} + Be^{-ikx}$$

For $x > 0$, $U = V_2$ and the SE becomes

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_2) \psi = 0$$

$$\psi = Ce^{ik_2x} + De^{-ik_2x}$$

where

$$k_2 = \frac{2m(E - V_2)}{\hbar}$$

At $x = 0$, ψ must be continuous

$$\psi(0-) = \psi(0+)$$

and

$$A + B = C + D$$

Now consider a particle incident from the left. For this case, we can set $D = 0$ and get that

$$A + B = C$$

Because $\frac{\partial\psi}{\partial x}$ is also required to be continuous,

$$ikA - ikB = ik_2C$$

or $k(A - B) = k_2C$, which can be expressed as $C = \frac{k}{k_2}(A - B)$.

Substituting in the previous expression yields

$$\begin{aligned}A + B &= \frac{k}{k_2}(A - B) \\A \left(1 - \frac{k}{k_2}\right) &= -B \left(1 + \frac{k}{k_2}\right) \\A \frac{k - k_2}{k_2} &= B \frac{k + k_2}{k_2} \\ \frac{B}{A} &= \frac{k - k_2}{k + k_2}\end{aligned}$$

and

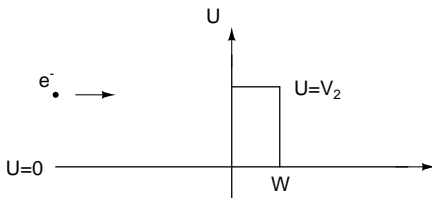
$$\frac{C}{A} = \frac{2k}{k + k_2}$$

Observations:

- If $E > V_2$,
 - both k and k_2 are real;
 - solutions are oscillatory;
 - $\frac{B}{A} = \frac{k-k_2}{k+k_2}$ is finite! Thus, there is a finite probability that the barrier will reflect back the electron, causing it to turn back to the left.
- If $E < V_2$,
 - $k_2 = \frac{2m(E-V_2)}{\hbar}$ is imaginary;
 - the wavefunction declines exponentially for $x > 0$.
 - $\frac{C}{A} = \frac{2k}{k+k_2} > 0$ so there is a non-zero probability for the electron to penetrate the barrier!

Tunneling

Consider an electron approaching the potential barrier of finite width:



An electron approaching a finite-width potential barrier.

- for $x < 0$ and for $x > W$
 - $\psi =$ free electron.
- for $0 \leq x \leq W$,
 - $\psi = \psi_2$ for a potential barrier.
- Thus,

$$\psi(x) = \begin{cases} A_+ e^{ikx} + A_- e^{-ikx} & \forall x < 0 \\ B_+ e^{ik_2x} + B_- e^{-ik_2x} & \forall 0 \leq x \leq W \\ C_+ e^{ikx} + C_- e^{-ikx} & \forall x > W \end{cases}$$

where $\hbar k = \sqrt{2mE}$ and $\hbar k_2 = \sqrt{2m(E - V_2)}$.

If an electron approaches the barrier from the left, $C_- = 0$.

Rather than proceeding to match the wave-functions and its derivative at $x = 0$ and $x = W$ to determine the relation between coefficients explicitly, we will just express the result in terms of the transmission coefficient, defined as

$$T = \left| \frac{C_+}{A_+} \right|^2$$

- For $E > V_2$,

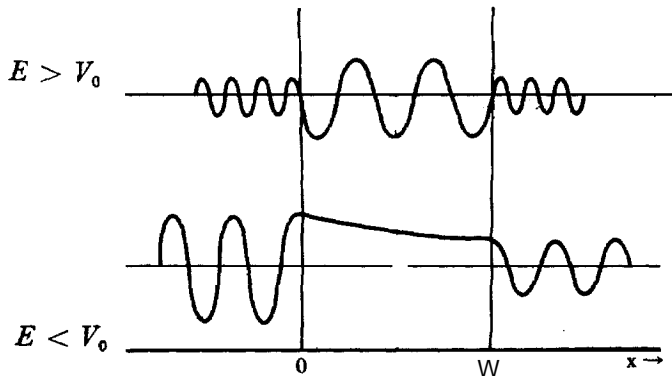
$$T = \frac{1}{1 + \frac{V_2^2}{4E(E-V_2)} S^2}$$

where $S = \sin(k_2 W)$. Notice that this equals unity for any barrier width for which $k_2 W = n\pi$, where n is any integer.

- For $E < V_2$,

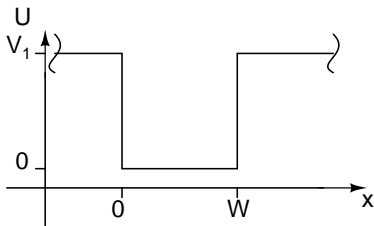
$$T = \frac{1}{1 + \frac{V_2^2}{4E(V_2-E)} S_h^2}$$

where $S = \sinh(ik_2 W)$.



ψ for the tunneling example. Observe that an electron with $E < V_2$ have a finite probability of penetrating the barrier.

Quantum Well



A one-dimensional quantum well.

Trial wave-functions:

$$\psi(x) = \begin{cases} A_1 e^{\alpha x} + B_1 e^{-\alpha x} & \forall x < 0 \\ A_0 \sin(kx) + B_0 \cos(kx) & \forall 0 \leq x \leq W \\ A_2 e^{\alpha x} + B_2 e^{-\alpha x} & \forall x > W \end{cases}$$

where

$$\alpha = \frac{\sqrt{2m(V_1 - E)}}{\hbar}$$

and

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

Observe that

- if $E > V_1$, α is imaginary and the corresponding exponential terms in the wave-function are oscillatory.
- if $E < V_1$, ψ should decay as it penetrates the barrier, and vanish far from it.
- This behavior requires that

$$B_1 = A_2 = 0$$

- The resulting wave-function is,

$$\psi(x) = \begin{cases} A_1 e^{\alpha x} & \forall x < 0 \\ A_0 \sin(kx) + B_0 \cos(kx) & \forall 0 \leq x \leq W \\ B_2 e^{-\alpha x} & \forall x > W \end{cases}$$

- Continuity boundary conditions at $x = 0$ and $x = W$:

$$\psi(0-) = \psi(0+) \quad \psi(W-) = \psi(W+)$$

$$\frac{d\psi}{dx}(0-) = \frac{d\psi}{dx}(0+)$$

$$\frac{d\psi}{dx}(W-) = \frac{d\psi}{dx}(W+)$$

- Solution is:

$$A_1 = B_0$$

$$B_0 = \frac{k}{\alpha} A_0$$

$$A_0 \sin(kW) + B_0 \cos(kW) = B_2 e^{-\alpha W}$$

$$k(A_0 \cos(kW) - B_0 \sin(kW)) = -\alpha B_2 e^{-\alpha W}$$

Solving B_2 , substituting and rearranging:

$$A_0 (k \cos(kW) + \alpha \sin(kW)) - B_0 (k \sin(kW) - \alpha \cos(kW)) = 0$$

After eliminating A_0 and B_0 ,

$$\tan(kW) = \frac{2k\alpha}{k^2 - \alpha^2}$$

In terms of a normalized energy $\xi = E/V_1$, and using

$$kW = \frac{\sqrt{2mE}}{\hbar} = \frac{W\sqrt{2mV_1}}{\hbar} \sqrt{\frac{E}{V_1}} = Wa\sqrt{\xi}$$

where $a = \frac{\sqrt{2mV_1}}{\hbar}$, and that

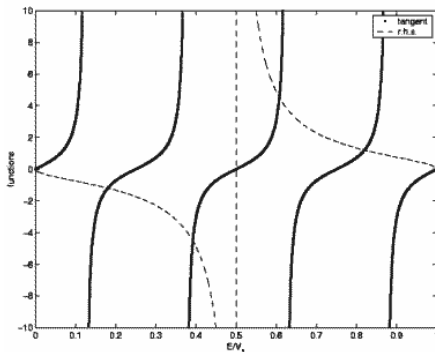
$$\frac{2k\alpha}{k^2 - \alpha^2} = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$

The solution becomes

$$\tan(Wa\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$

Observe that:

- The tangent of θ increases from 0 at $\theta = 0$ to $+\infty$ at $\theta = \pi/2$;
- it then jumps discontinuously to $-\infty$ and increases again to 0 at $\theta = \pi$.
- This behavior repeats with a period π .



Comparison of the two sides of the result obtained for the quantum well, for $Wa = 4\pi$. The two expressions intercept at four energy levels, for which the particle is confined in the well.