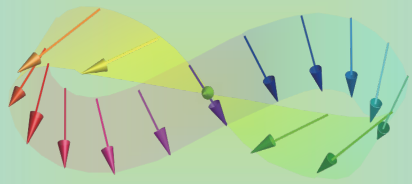
Nanoelectronics
07



Atsufumi Hirohata

Department of Electronic Engineering

THE UNIVERSITY of York

09:00 Thursday, 09/February/2023 (P/T 005A)

Quick Review over the Last Lecture

Schrödinger equation :

( )

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2}\psi = (\boxed{E} - V)\psi$$

( ) ( )

For example,

$$-i\hbar\frac{\partial}{\partial x}e^{inx} = \hbar n e^{inx}$$

$\hbar n$ ( )

e^{inx} ( )

$$\int \left(H\psi(x,t)\right)^* \psi(x,t)dx = \int \psi^*(x,t)H\psi(x,t)dx$$

$\rightarrow H$: ( )

Ground state still holds a minimum energy :

$$E = \frac{\pi^2\hbar^2}{2mL^2} \neq 0 \quad \rightarrow (\quad)$$

Contents of Nanoelectonics

05 Quantum Well

- 1D quantum well
- Quantum tunnelling

Classical Dynamics / Quantum Mechanics

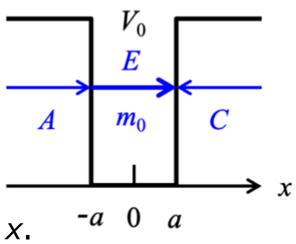
Major parameters :

Quantum mechanics	Classical dynamics
equation	
ψ :	A :
$\|\psi\|^2$:	A^2 :

1D Quantum Well Potential

A de Broglie wave (particle with mass m_0) confined in a square well :

$$\begin{cases} \dfrac{\hbar^2}{2m_0}\dfrac{d^2\psi_1}{dx^2} + (E - V_0)\psi_1 = 0 \quad (\qquad\qquad) \\ \dfrac{\hbar^2}{2m_0}\dfrac{d^2\psi_2}{dx^2} + E\psi_2 = 0 \quad (\qquad\qquad) \end{cases}$$



For $E > V_0$, a general solution is obtained for $x < -a$ and $a < x$.

$$\frac{\hbar^2}{2m_0}\frac{d^2\psi_1}{dx^2} = -(E - V_0)\psi_1$$

$$-\frac{\hbar^2}{2m_0}\psi_1'' = (E - V_0)\psi_1$$

$$\therefore \psi_1'' = \frac{2m_0(E - V_0)}{\hbar^2}\psi_1.$$

Hence, a general solution for the wave function ψ_1 is $k_1 =$.

Similarly, for $-a \le x \le a$, a general solution for the wave function ψ_2 is

$k_2 =$.

1D Quantum Well Potential (Cont'd)

Accordingly, the wave functions can be defined as

$$\begin{cases} \psi_1 = A_1\exp(ik_1x) + A_2\exp(-ik_1x) & (x < -a) \\ \psi_2 = B_1\sin(k_2x) + B_2\cos(k_2x) & (-a \le x \le a) \\ \psi_1 = C_1\exp(ik_1x) + C_2\exp(-ik_1x) & (a < x) \end{cases}$$

For most of nanoelectronic devices, $E < V_0$, meaning that k_1 becomes imaginary.

Hence, the general solution for the wave function ψ_1 is defined as ${k_1}' =$

which satisfies $ik_1 = {k_1}'$.

By replacing k_1 with $i{k_1}'$ in the above equations,

$$\begin{cases} \psi_1 = & (x < -a) \\ \psi_2 = & (-a \le x \le a) \\ \psi_1 = & (a < x) \end{cases}$$

Since the particle is confined in the well, $\psi_1 \to 0$ at $x \to \pm\infty$, resulting in

$A_2 =$ and $C_1 =$.

1D Quantum Well Potential (Cont'd)

Now, boundary conditions at x = -a and a are

$$\begin{cases} \psi_1(-a) = \psi_2(-a) \\ {\psi_1}'(-a) = {\psi_2}'(-a) \\ \psi_2(a) = \psi_1(a) \\ {\psi_2}'(a) = {\psi_1}'(a) \end{cases}$$

$$\therefore \begin{cases} \\ \\ \\ \end{cases}$$

By rearranging these conditions,

$$\begin{cases} 2B_1\sin(k_2a) = (C_2 - A_1)\exp(-{k_1}'a) \\ 2k_2B_1\sin(k_2a) = -k_1(C_2 - A_1)\exp(-{k_1}'a) \\ 2B_2\cos(k_2a) = (C_2 + A_1)\exp(-{k_1}'a) \\ 2k_2B_1\cos(k_2a) = k_1(C_2 + A_1)\exp(-{k_1}'a) \end{cases}$$

1D Quantum Well Potential (Cont'd)

For $B_1 \neq 0$ and $C_2 - A_1 \neq 0$,

.

For $B_2 \neq 0$ and $C_2 + A_1 \neq 0$,

.

Here, for $B_1 \neq 0$ and $B_2 \neq 0$, $\tan^2(k_2 a) = -1$, resulting in k_2 to be an imaginary figure, which cannot satisfy the Schrödinger equations.

Accordingly, either $B_1 \neq 0$ or $B_2 \neq 0$ can satisfy the equations.

(i) For $B_1 = 0$ and $B_2 \neq 0$, $A_1 = C_2$ leading to

. (1)

(ii) For $B_1 \neq 0$ and $B_2 = 0$, $A_1 = -C_2$ leading to

. (2)

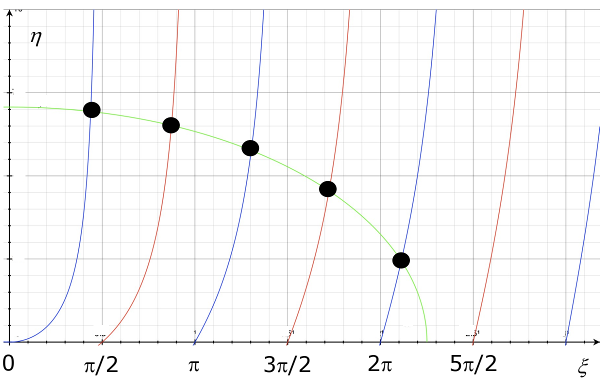
Note that $k_1{}' = \frac{\sqrt{2m_0(V_0 - E)}}{\hbar}$ and $k_2 = \frac{\sqrt{2m_0 E}}{\hbar}$, which give

$$(k_1{}')^2 + k_2{}^2 = \frac{2m_0 V_0}{\hbar^2}$$

∴ . (3)

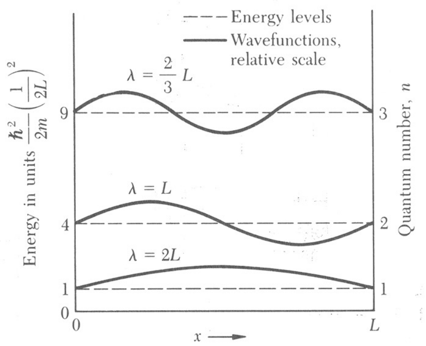
1D Quantum Well Potential (Cont'd)

Therefore, the answers for $k_2 a (= \xi)$ and $k_1{}' a (= \eta)$ are crossings of the Eqs. (1) / (2) and (3).



Energy eigenvalues are also obtained as

→ Discrete states

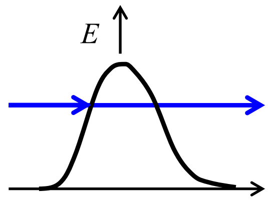


* C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, New York, 1986).

Quantum Tunnelling

In classical theory,

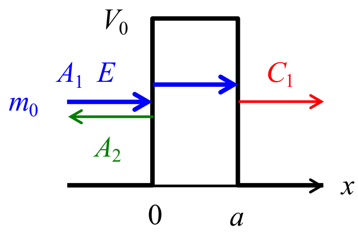
Particle with smaller energy than the potential barrier cannot pass through the barrier.



In quantum mechanics, such a particle have probability to tunnel.

For a particle with energy E ($< V_0$) and mass m_0,

Schrödinger equations are



$$\begin{cases} \dfrac{\hbar^2}{2m_0}\dfrac{d^2\psi}{dx^2} + E\psi = 0 & (x < 0, a < x) \\ \dfrac{\hbar^2}{2m_0}\dfrac{d^2\psi}{dx^2} + (E - V_0)\psi = 0 & (0 < x < a) \end{cases}$$

Substituting general answers $k_1 = \sqrt{2m_0E}/\hbar$, $k_2 = \sqrt{2m_0(V_0 - E)}/\hbar$

$$\begin{cases} \psi = \boxed{A_1 \exp(ik_1x)} + \boxed{A_2 \exp(-ik_1x)} & (x < 0) \\ \psi = B_1 \exp(k_2x) + B_2 \exp(-k_2x) & (0 < x < a) \\ \psi = \boxed{C_1 \exp(ik_1x)} & (a < x) \end{cases}$$

Quantum Tunnelling (Cont'd)

Now, boundary conditions are

$$\begin{cases} A_1 + A_2 = B_1 + B_2,\ \ ik_1(A_1 - A_2) = k_2(B_1 - B_2) & (x = 0) \\ B_1 \exp(k_2a) + B_2 \exp(-k_2a) = C_1 \exp(ik_1a),\ \ k_2[B_1 \exp(k_2a) - B_2 \exp(-k_2a)] = ik_1C_1 \exp(ik_1a) & (x = a) \end{cases}$$

$$\therefore \begin{cases} \dfrac{A_2}{A_1} = \dfrac{(k_1{}^2 + k_2{}^2)\{\exp(k_2a) - \exp(-k_2a)\}}{(k_2{}^2 - k_1{}^2)\{\exp(k_2a) - \exp(-k_2a)\} - 2ik_1k_2\{\exp(k_2a) + \exp(-k_2a)\}} \\ \dfrac{C_1}{A_1} = \dfrac{4k_1k_2\exp(-ik_1a)}{(k_2{}^2 - k_1{}^2)\{\exp(k_2a) - \exp(-k_2a)\} - 2ik_1k_2\{\exp(k_2a) + \exp(-k_2a)\}} \end{cases}$$

By using the following relationships: $\exp(k_2a) - \exp(-k_2a)/2 = \sinh(k_2a)$ and $\exp(k_2a) + \exp(-k_2a)/2 = \cosh(k_2a)$, transmittance T and reflectance R are

$$\begin{cases} R = \left|\dfrac{A_2}{A_1}\right|^2 = \dfrac{V_0{}^2 \cdot \sinh^2\left(\dfrac{\sqrt{2m_0(V_0 - E)}}{\hbar}a\right)}{V_0{}^2 \cdot \sinh^2\left(\dfrac{\sqrt{2m_0(V_0 - E)}}{\hbar}a\right) + 4E(V_0 - E)} \\ T = \left|\dfrac{C_1}{A_1}\right|^2 = \dfrac{4E(V_0 - E)}{V_0{}^2 \cdot \sinh^2\left(\dfrac{\sqrt{2m_0(V_0 - E)}}{\hbar}a\right) + 4E(V_0 - E)} \end{cases}$$

→ →

Quantum Tunnelling (Cont'd)

For $V_0 - E \gg \hbar^2/2m_0a^2$,

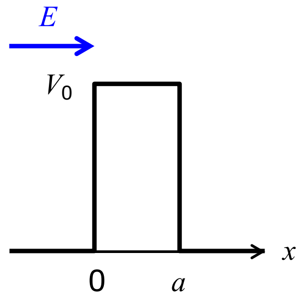
$$\hbar^2/a \ll \sqrt{2m_0(V_0 - E)}$$

$$\therefore V_0{}^2 \cdot \sinh^2\left(\frac{\sqrt{2m_0(V_0 - E)}}{\hbar}a\right) \approx V_0{}^2 \cdot \exp\left(\frac{\sqrt{2m_0(V_0 - E)}}{\hbar}a\right)$$

$$\therefore T \approx \frac{4E(V_0 - E)}{V_0{}^2}\exp\left(-\frac{\sqrt{2m_0(V_0 - E)}}{\hbar}a\right)$$

→ *T* exponentially decrease with increasing *a* and (V_0 - *E*)

For $V_0 < E$, as k_2 becomes an imaginary number, k_2 should be substituted with



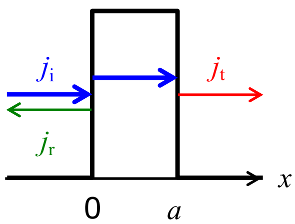
$$k_2{}' = \frac{\sqrt{2m_0(E - V_0)}}{\hbar} \quad (k_2 \to ik_2{}')$$

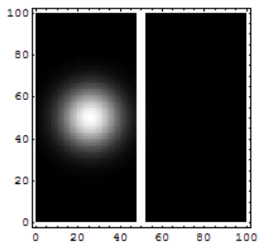
$$\therefore \begin{cases} R = \left|\frac{A_2}{A_1}\right|^2 = \frac{\left(k_1{}^2 - k_2{}^2\right)^2 \cdot \sin^2(k_2a)}{\left(k_1{}^2 - k_2{}^2\right)^2 \cdot \sin^2(k_2a) + 4k_1{}^2k_2{}^2} \\ T = \left|\frac{C_1}{A_1}\right|^2 = \frac{4k_1{}^2k_2{}^2}{\left(k_1{}^2 - k_2{}^2\right)^2 \cdot \sin^2(k_2a) + 4k_1{}^2k_2{}^2} \end{cases}$$

→

Quantum Tunnelling - Animation

Animation of quantum tunnelling through a potential barrier





* http://www.wikipedia.org/

Absorption Coefficient

Absorption fraction A is defined as

Here, $j_r = Rj_i$, and therefore $(1 - R)\, j_i$ is injected.

Assuming j at x becomes $j - dj$ at $x + dx$,

$$-dj = \alpha j dx \qquad (\alpha : \text{absorption coefficient})$$

With the boundary condition : at $x = 0$, $j = (1 - R)\, j_i$,

$$j = (1 - R)\, j_i \exp(-\alpha x)$$

With the boundary condition : $x = a$, $j = (1 - R)\, j_i e^{-\alpha a}$,

part of which is reflected ; $R\,(1 - R)\, j_i\, e^{-\alpha a}$

and the rest is transmitted ; $j_t = [1 - R - R\,(1 - R)]\, j_i\, e^{-\alpha a}$

$$j_t = (1 - R)^2 j_i \exp(-\alpha x)$$

$$\therefore T = \frac{j_t}{j_i} = (1 - R)^2 \exp(-\alpha x)$$