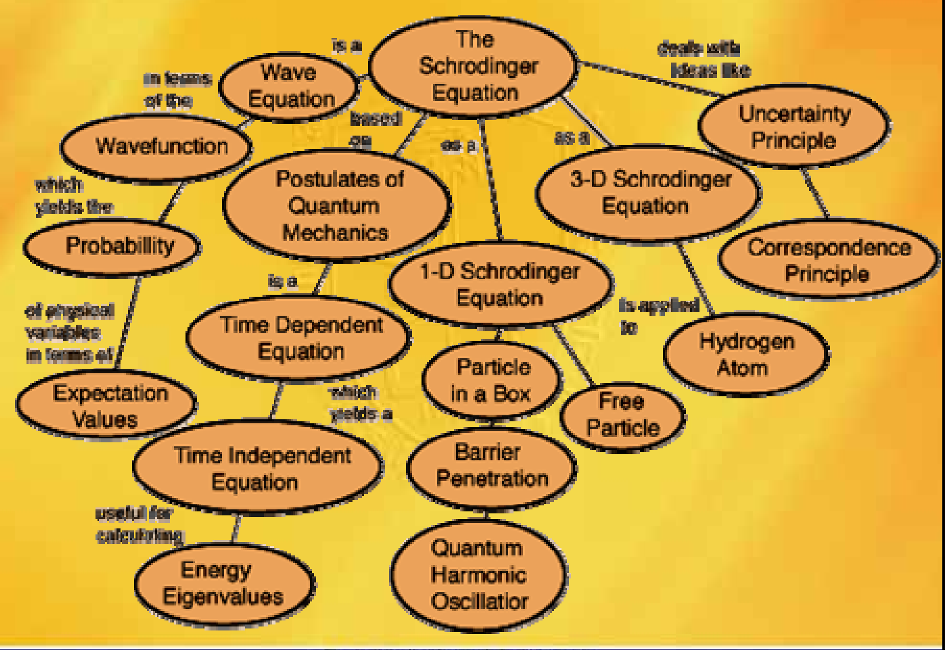

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The Time – independent Schrödinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Time-dependent Schrödinger wave eq

دالة شرودنجر المعتمدة علي الزمن

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Time-independent Schrödinger equation
معادلة شرودنجر الغير معتمده على الزمن

عندما يكون النظام في حالة إستقرار stationary فإن ذلك يعني انه لايتغير مع الزمن.

نفترض أن الجهد V لايعتمد على الزمن

$$V(x,t)=V(x)$$

وبالنظر الى معادلة شرودنجر يلاحظ:

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

الطرف الأيسر (LHS) يحتوى فقط على تغيير Ψ مع t

الطرف الأيمن (RHS) يحتوى فقط على تغير Ψ مع x (أي أن مؤثر هاملتون لايعتمد على الزمن t

للحصول على معادلة شرودنجر يستخدم فصل المتغيرات separation of variables

$$\Psi(x,t)=\psi(x)T(t)$$

حيث $\psi(x)$ دالة تعتمد على المكان فقط و $T(t)$ دالة تعتمد على الزمن فقط .

وبالتعويض في معادلة شرودنجر:

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

$$\frac{\partial^2}{\partial x^2}[\psi(x)T(t)]=T(t)\frac{d^2\psi}{dx^2} \quad \text{etc}$$

لاحظ هنا التفاضل كلي Total وليس جزئي partial derivative

$$-\frac{\hbar^2}{2m}T\frac{d^2\psi}{dx^2}+V(x)\psi T=i\hbar\psi\frac{dT}{dt} \qquad (3)$$

$$-\frac{\hbar^2}{2m}T\frac{d^2\psi}{dx^2}+V(x)\psi T=i\hbar\psi\frac{dT}{dt}$$

بالقسمة على $T\psi$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2}+V(x)=i\hbar\frac{1}{T}\frac{dT}{dt} \qquad (4)$$

الطرف الأيسر يعتمد على x و الطرف الأيمن يعتمد على t

وهذا صحيح لجميع x و t وبالتالي يجب أن يساوي الطرفين مقدار ثابت E (E تسمي ثابت الفصل)

$$i\hbar\frac{1}{T}\frac{dT}{dt}=E \qquad (5)$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2}+V(x)=E \qquad (6)$$

لدينا الآن معادلتين ، واحدة تعتمد فيها الدالة الموجية على الزمن والأخري تعتمد الدالة الموجية على المكان .

كيف نجد ثابت الفصل E ؟

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$$i\hbar\frac{1}{T}\frac{dT}{dt}=E \;\Rightarrow\; \frac{dT}{T}=\left(\frac{-iE}{\hbar}\right)dt$$

$$\int\frac{dT}{T}=\left(\frac{-iE}{\hbar}\right)\int dt \;\Rightarrow\; \ell n\ T=\frac{-iE}{\hbar}t$$

$$T(t)=e^{-i(E/\hbar)t} \qquad (7)$$

لاحظ أن المقدار $(E/\hbar)$ يجب أن يكون له وحدة مقلوب الزمن لكي تصبح الأسية بدون وحدة .

ولكن:

$(E/\hbar)\rightarrow 1/s \Longrightarrow$ unit of E=unit of $\hbar$/s =J.s/s=J

إذاً يجب أن تكون وحدة E هي الجول (J)

وبالتالي يكون ثابت الفصل هو الطاقة E

$$E=\hbar\omega$$

$$T(t)=e^{-iEt/\hbar}=e^{-i\omega t} \qquad (8)$$

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$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2}+V(x)=E \qquad (6)$$

بضرب المعادلة (6) في ψ نجد أن:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+V(x)\psi=E\psi \qquad (9)$$

ويمكن كتابة معادلة شرودنجر الغير معتمدة على الزمن (TISE) على الصورة:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+\frac{2m}{\hbar^2}[E-V(x)]\psi=0 \qquad (10)$$

$$\nabla^2\psi(x,y,z)+\frac{2m}{\hbar^2}[E-V(x,y,z)]\psi(x,y,z)=0 \qquad (11)$$

$$\hat{H}\psi=E\psi \qquad (12)$$

والحل الكامل لمعادلة شرودنجر المعتمدة على الزمن (TDSE) يكون على الصورة:

$$\Psi(x,t)=\psi(x)T(t)=\psi(x)e^{-iEt/\hbar}$$

بالرغم من أن الجهد لايعتمد على الزمن فإن الدالة الموجية لاتزال تهتز كدالة في الزمن

SUMMARY
ملخص

معادلة شرودنجر المعتمدة علي الزمن (TISE)

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

الإحتمالية **Probability** والتعاير **normalization**

$$P(x,t)dx=\left|\Psi(x,t)\right|^2 dx=\Psi^*(x,t)\Psi(x,t)dx$$

$$\int_{-\infty}^{+\infty} dx\, P(x,t)=\int_{-\infty}^{+\infty} dx\left|\Psi(x,t)\right|^2=1$$

معادلة شرودنجر الغير معتمدة علي الزمن (TISE)

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

$$\Psi(x,t)=\psi(x)T(t)=\psi(x)e^{-iEt/\hbar}$$

شروط الدالة الموجية:
قيمة واحدة ومتصلة ومتعامدة
ومتصلة عند تفاضلها الأول

حل معادلة شرودنجر الغير معتمدة على الزمن TISE

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left[E-V(x)\right]\psi=0$$

(1) لجسيم حر حيث $V(x) = V_0 = 0$

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}E\psi=0$$

حلها على الصورة:

$$\psi(x) = Ne^{\pm i\sqrt{2mE/\hbar^2}}$$

حيث N يمثل ثابت التعاير .

(2) لجسيم يتحرك في جهد مقداره V_0 حيث $E > V_0$

$$\psi(x) = Ae^{ikx}+Be^{-ikx} = A'\sin kx + B'\cos kx$$

حيث $k=\sqrt{\frac{2m(V_o-E)}{\hbar^2}}$ و A, B, A', B' ثوابت .

(2) لجسيم يتحرك في جهد مقداره V_0 حيث $E > V_0$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad k = \sqrt{\frac{2m(E - V_o)}{\hbar^2}}$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx} = A'\sin kx + B'\cos kx$$

حيث A, B, A', B' ثوابت .

(3) لجسيم يتحرك في جهد مقداره V_0 حيث $E < V_0$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[V_0 - E]\psi = 0$$

$$\frac{d^2\psi}{dx^2} - k^2\psi = 0 \qquad k = \sqrt{\frac{2m(E - V_o)}{\hbar^2}}$$

$$\psi(x) = Ce^{k_2 x} + De^{-k_2 x}$$

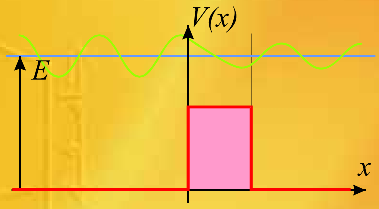
حيث C,D ثوابت .

إن النتائج التى تم الحصول عليها بواسطة معادلة شرودنجر تختلف عن النتائج التى تم الحصول عليها بواسطة الميكانيا التقليدية:

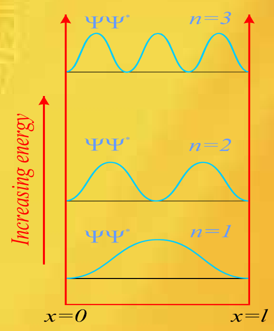
(1) توقعت ميكانيكا الكم حالات الطاقة المنفصلة discrete energy states في حين توقعت الميكانيكا التقليدية مدى الطاقات المستمرة.

تطبيقات على معادلة شرودنجر
Applications: simple systems

- Potential wells
  - Stationary states
    - atoms (crude model)
    - electrons in metals (surprisingly good model)

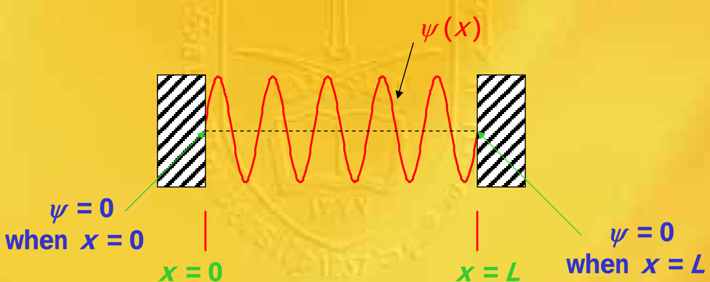


- Potential barriers
  - Tunnelling
    - radioactive decay



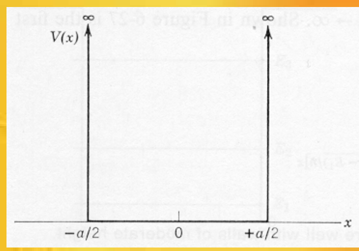
- Potential steps
  - Scattering
    Boundary conditions at a potential discontinuity

- Boundary conditions at a potential discontinuity
  - (1) The wavefunction, Ψ, is continuous
  - (2) The gradient , $d\Psi/dx$, is continuous



The Infinite Square Well potential

$$V(x) = \begin{cases} \infty & x < -a/2 \text{ or } x > a/2 \\ 0 & -a/2 < x < a/2 \end{cases}$$



For $-a/2 < x < a/2$ the general solution is still

$\psi(x) = A\sin kx + B\cos kx$ where $k = \frac{\sqrt{2mE}}{\hbar}$

What are the boundary conditions ? $\psi(x) = 0$ at $x = \pm a/2$

$A\sin(-ka/2) + B\cos(-ka/2) = 0$

$A\sin(ka/2) + B\cos(ka/2) = 0$

adding, we find $2B\cos(ka/2) = 0$

subtracting we find $2A\sin(ka/2) = 0$

Since we require that A or B be different from zero, we get two classes of solutions:

Class One: $A = 0$, $\cos(ka/2) = 0$

$\psi(x) = B\cos(kx)$

$ka/2 = \pi/2, 3\pi/2, 5\pi/2, \ldots$

$k_n = n\pi/a$, n odd

Class Two: $B = 0$, $\sin(ka/2) = 0$

$\psi(x) = A\sin(kx)$

$ka/2 = n\pi$

$k_n = n\pi/a$, n even $\neq 0$.

$$E_n = \frac{p_n^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

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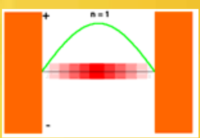
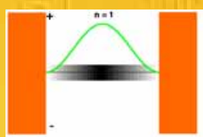
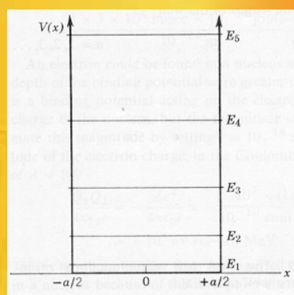
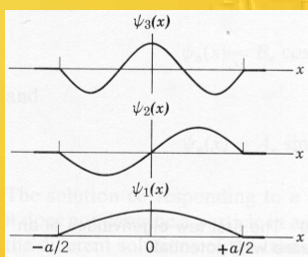
$$E_n = \frac{p_n^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

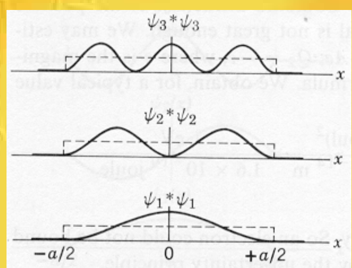
consider E_1: This is the lowest energy – the particle cannot have zero energy – basically due to the uncertainty principle. Equivalently, there must be zero-point energy because there must be zero-point motion





Note alternating parity! (again)



compare classical (dashed) with QM

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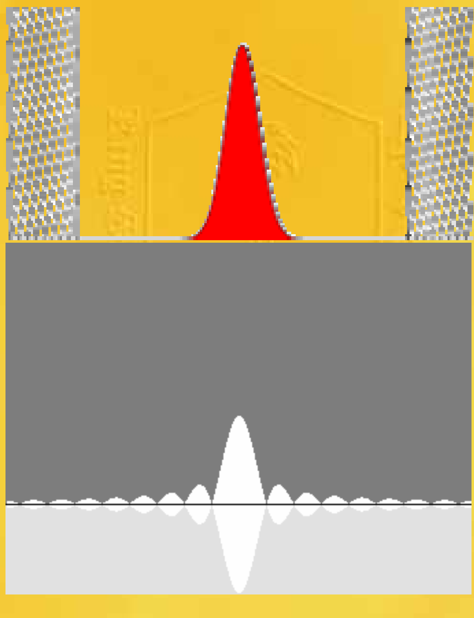
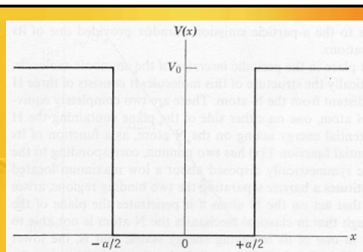


The Square Well potential

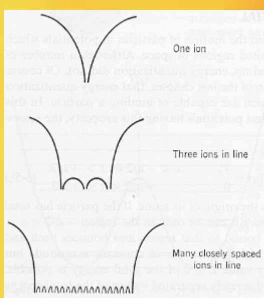
$$V(x) = \begin{cases} V_0 & x < -a/2 \text{ or } x > a/2 \\ 0 & -a/2 < x < a/2 \end{cases}$$



What do we expect classically ?

If $E < V_0$ then classically (i) the particle will be bound to the well, if $E \geq V_0$ particle is free…

Many systems can be approximated with a square well potential (i.e. many closely space ions in a line)



The general solution of Schrödinger's equation inside the well is

$$\psi(x) = Ae^{ik_I x} + Be^{-ik_I x} \qquad \text{where} \qquad k_I = \frac{\sqrt{2mE}}{\hbar}$$

Alternatively, the two independent solutions can be written as

$\psi(x) = B'\cos k_I x$ and $\psi(x) = A'\sin k_I x$ so the general solution is

$$\psi(x) = A'\sin k_I x + B'\cos k_I x$$

Outside the well, for $E < V_0$, we have

$$\psi(x) = Ce^{k_{II} x} + De^{-k_{II} x} \quad x < -a/2$$

$$\psi(x) = Fe^{k_{II} x} + Ge^{-k_{II} x} \quad x > a/2$$

$$k_{II} = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

What can we immediately say about D and F ? Both zero

As usual, the relations between A’, B’, C, and G are determined by the continuity of ψ and $d\psi/dx$ at $x = \pm a/2$

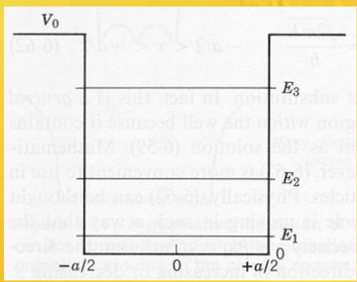
So, we now have 4 equations and only 4 unknowns – this is a problem. Why ?

We need to leave one constant free for amplitude (and so we can satisfy the normalization condition)

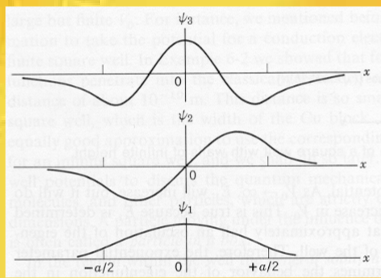
To solve this, we treat the total energy as an additional constant that can be adjusted as necessary (where we will find that E can only take on certain values)

The general solution to the square-well potential is quite complex and involves a transcendental equation – see Appendix H

three bound eigenvalues



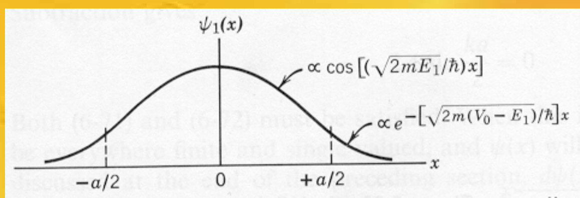
three bound eigenfunctions



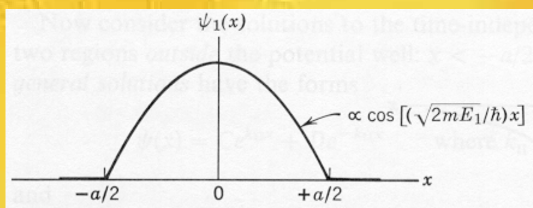
Note alternating parity!

Before moving onto the next section, it is instructive to consider what happens as we let V_0 becomes very large

moderate height



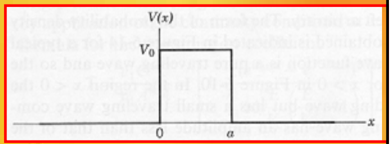
infinite height



The Barrier potential

So what's a barrier potential ?

$$V(x) = \begin{cases} V_0 & 0 < x < a \\ 0 & x < 0,\ x > a \end{cases}$$



Classically what do we expect for particle traveling in the $+x$ direction towards $x = 0$?

If $E < V_0$, particle bounces back, if $E > V_0$, particle passes barrier, slow down in $0 < x < a$, speed up $x > a$

Quantum mechanically we find tunneling through the barrier when $E < V_0$, with a probability which

(a) increases as $E - V_0$ increases and (b) decreases as a increases.

(b) We will also find that inside the barrier $\psi(x)$ decays exponentially.

In the next section we will consider several tunneling phenomena in detail
in this section we solve Schrödinger's equation for $\psi(x)$

Looking first at the regions $x < 0$ and $x > a$, what are the general solutions ?

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x < 0 \\ Ce^{ik_1x} + De^{-ik_1x} & x > a \end{cases} \qquad \text{where} \qquad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

And since there is no particle moving in $x > a$ towards $x < a$, what can we say about D ? $D = 0$

What info do we need before we can write down the general solution for the region $0 < x < a$?

Whether $E < V_0$ or $E > V_0$ We've already examined both cases – let's start with $E < V_0$

So what's the general solution in the region $0 < x < a$ with $E < V_0$?

$$\psi(x) = Fe^{-k_2x} + Ge^{+k_2x} \qquad \text{where} \qquad k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

What are our continuity conditions ?

$$A + B = F + G$$

$$ik_1(A - B) = k_2(-F + G)$$

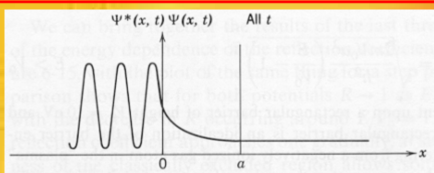
$$Ce^{ik_1a} = Fe^{-k_2a} + Ge^{+k_2a}$$

$$ik_1Ce^{ik_1a} = k_2\{Ge^{+k_2a} - Fe^{-k_2a}\}$$

As expected, we have indeed 4 linear equations in the 5 unknowns *A, B, C, F,* and *G.*

To solve, first express F and G in terms of A and B, then C in terms of A and B, then finally B in terms of A

What does $\Psi^*\Psi$ look like ?

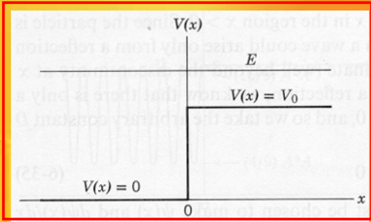


For T we find $T = \frac{v_1 C^* C}{v_1 A^* A} = \left[1 + \frac{\left(e^{k_2a} - e^{-k_2a}\right)^2}{16(E/V_0)(1 - E/V_0)}\right]^{-1} = \left[1 + \frac{\sinh^2 k_2a}{4(E/V_0)(1 - E/V_0)}\right]^{-1}$

and if $k_2a \gg 1$ then $T \approx 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2k_2a}$

T decreases exponentially with increasing barrier width a. The last two results provide the essence of barrier penetration or *tunneling phenomena,* which are purely quantum mechanical

The Step potential: energy > step height



First question: what happens to a classical particle ?

A *particle* moving in the $+x$ direction will simply slow down at $x = 0$, from $v_1 = p_1/m = [2E/m]^{1/2}$ to $v_2 = p_2/m = [2(E - V_0)/m]^{1/2}$

What happens to a wave ?

A *wave* traveling in the $+x$ direction and passing from the first medium to the second medium will be partially reflected and partially transmitted

So, the quantum mechanical interpretation for a particle would be … ?

The particle has a certain probability T of being transmitted and a probability $R = 1 - T$ of being reflected

The general solution here is, of course, the same as for the $x < 0$ part of the $E < V_0$ case, who remembers ?

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x < 0 \\ Ce^{ik_2x} + De^{-ik_2x} & x > 0 \end{cases} \quad \text{where} \quad k_1 = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

Noting
- the physical meaning of each term
- that the particle is moving from $x < 0$ towards $x > 0$
- that there is no particle moving in $x > 0$ towards $x < 0$

What can we say about D ? $D = 0$?

And from the continuity of $\psi(x)$ at $x = 0$ what constraint do we have ? $A + B = C$

What do we get from the continuity of $d\psi(x)/dx$ at $x = 0$? $ik_1(A - B) = ik_2C$ ⇨ $A - B = k_2/k_1\, C$

Adding these two equations we get $A = \left(1 + \frac{k_2}{k_1}\right)\frac{C}{2} = \left(\frac{k_1 + k_2}{k_1}\right)\frac{C}{2}$ ⇨ $C = \frac{2k_1}{k_1 + k_2}A$

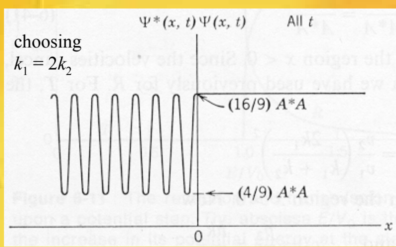
And subtracting $B = \left(1 - \frac{k_2}{k_1}\right)\frac{C}{2} = \left(\frac{k_1 - k_2}{k_1}\right)\frac{C}{2}$ ⇨ $B = \frac{k_1 - k_2}{k_1 + k_2}A$

For $x \le 0$, what does the first term represent ?
incident particle
and the second term ?
reflected particle

For $x \ge 0$, what does the only term represent ?
transmitted particle

$$\psi(x) = \begin{cases} Ae^{ik_1x} + A\frac{k_1 - k_2}{k_1 + k_2}e^{-ik_1x} & x \le 0 \\ A\frac{2k_1}{k_1 + k_2}e^{ik_2x} & x \ge 0 \end{cases}$$

So, what does $P(x,t) = \Psi^*\Psi$ look like ?



$x \le 0$: combination of a traveling plane wave + oscillatory standing wave
$x \ge 0$: traveling plane wave

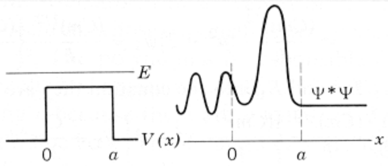
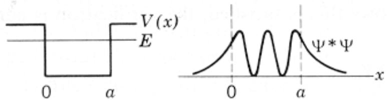
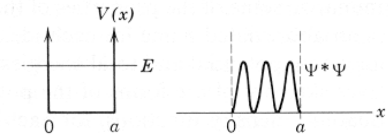
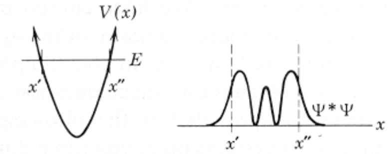
The reflection coefficient R is

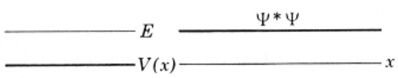
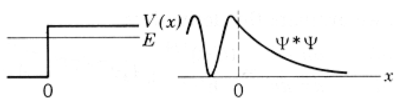
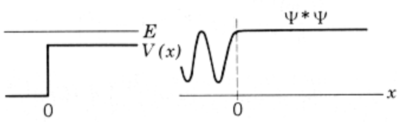
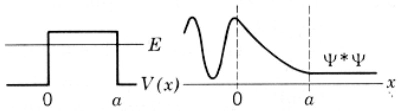
$$R = \frac{B^*B}{A^*A} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

is < 1 when $k_2 < k_1$ $(E > V_0)$

The transmission probability is $T = 1 - R = \frac{4k_1k_2}{(k_1 + k_2)^2} \ne \frac{C^*C}{A^*A}$

woops! Why doesn't T equal $\frac{C^*C}{A^*A}$?

Name of System	Physical Example	Potential and Total Energies	Probability Density	Significant Feature
Barrier potential (energy above top)	Electron scattering from negatively ionized atom			No reflection at certain energies
Finite square well potential	Neutron bound in nucleus			Energy quantization
Infinite square well potential	Molecule strictly confined to box			Approximation to finite square well
Simple harmonic oscillator potential	Atom of vibrating diatomic molecule			Zero-point energy

Name of System	Physical Example	Potential and Total Energies	Probability Density	Significant Feature
Zero potential	Proton in beam from cyclotron			Results used for other systems
Step potential (energy below top)	Conduction electron near surface of metal			Penetration of excluded region
Step potential (energy above top)	Neutron trying to escape nucleus			Partial reflection at potential discontinuity
Barrier potential (energy below top)	α particle trying to escape Coloumb barrier			Tunneling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