In this Chapter we will focus on solutions of the time-independent Schrödinger equation for various potentials.

The Free Particle: $V(x) = 0$.

The wavefunction for the free particle will have the following form:

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

where E is the total energy of the particle. The position dependent component of the wavefunction must satisfy the following differential equation

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

The general solution of this equation is

$$\psi(x) = e^{\pm ikx}$$

In order for this function to be a solution we must require that

$$-\frac{\hbar^2}{2m}\frac{\partial^2\left(e^{\pm ikx}\right)}{\partial x^2} = -\frac{\hbar^2}{2m}(\pm ik)^2 e^{\pm ikx} = \frac{\hbar^2 k^2}{2m}e^{\pm ikx} = Ee^{\pm ikx} \quad \Rightarrow \quad k = \frac{\sqrt{2mE}}{\hbar}$$

The general solution of the Schrödinger equation for a free particle is thus given by

$$\Psi(x,t) = \left(Ae^{+ikx} + Be^{-ikx}\right)e^{-i\omega t} = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$$

The first term of the solution represents a particle moving towards larger x. Consider for example the position of the maximum of the real component of this term at time t. The position of the maximum, x, must satisfy the following requirement:

$$kx - \omega t = 2\pi n$$

or

$$x = \frac{2\pi n + \omega t}{k}$$

When we look at the position of the maximum at time $t + dt$ we observe that is has move to a position $x + dx$ where

$$x+dx=\frac{2\pi n+\omega(t+dt)}{k}=\frac{2\pi n+\omega t}{k}+\frac{\omega dt}{k}=x+\frac{\omega dt}{k}\quad\Rightarrow\quad dx=\frac{\omega dt}{k}$$

Since $dt > 0$ we conclude that $dx > 0$. The maximum thus moves towards larger x. We conclude that

$$\Psi(x,t)=Ae^{i(kx-\omega t)}:\quad \text{wave travelling to the right}$$
$$\Psi(x,t)=Be^{i(-kx-\omega t)}:\quad \text{wave travelling to the left}$$

Consider first the case where $B = 0$. The probability distribution associated with the eigenfunction is equal to

$$P(x,t)=\Psi^*(x,t)\Psi(x,t)=\left(A^*e^{-i(kx-\omega t)}\right)\left(Ae^{i(kx-\omega t)}\right)=A^*A$$

The integral of the probability distribution must be equal to 1 and this requires that

$$\int_{-\infty}^{\infty}P(x,t)dx=\int_{-\infty}^{\infty}A^*A\,dx=A^*A\int_{-\infty}^{\infty}dx=1$$

But the integral of dx will approach infinity and A^*A must approach 0. However, in reality there are limits on the range of x and the integral of dx is thus finite. As a consequence A^*A is non-zero.

The momentum of the particle can be determined by calculating the expectation value of p:

$$\begin{aligned}\bar{p}\quad &=\langle p\rangle=\langle\Psi|p\Psi\rangle=\int\Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi\,dx=A^*A\int e^{-i(kx-\omega t)}\left(-i\hbar\frac{\partial}{\partial x}\right)e^{i(kx-\omega t)}\,dx=\\ &=A^*A\big((-i\hbar)(ik)\big)\int e^{-i(kx-\omega t)}e^{i(kx-\omega t)}\,dx=(\hbar k)A^*A\int dx=\hbar k\end{aligned}$$

The expectation value of p is thus equal to

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

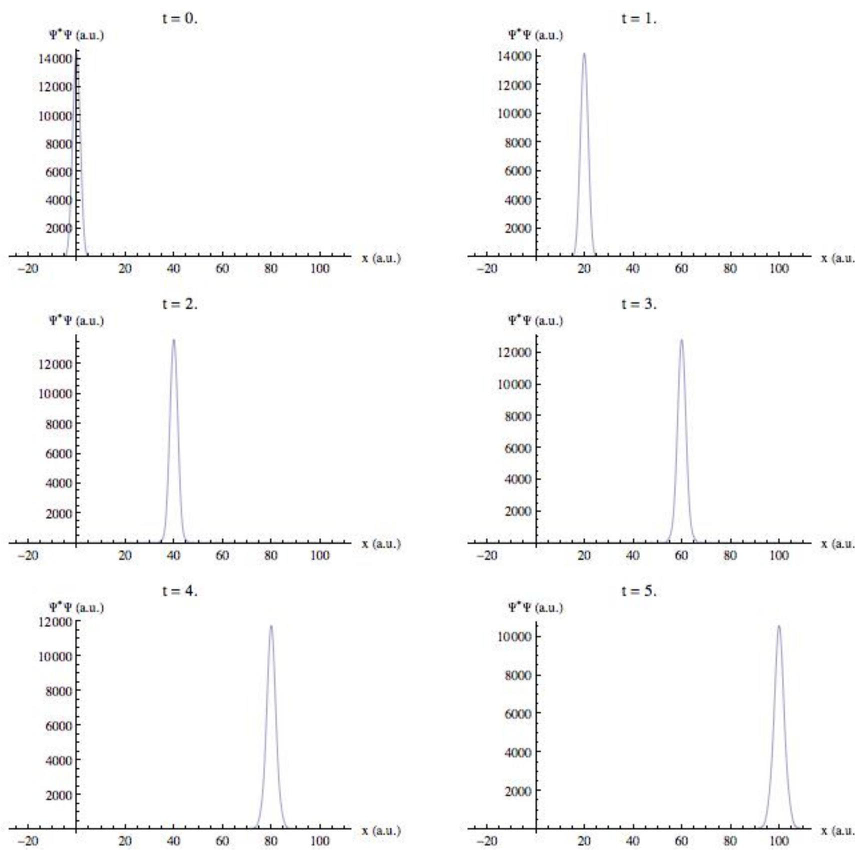
We thus conclude that $Ae^{i(kx-\omega t)}$ represents a particle of momentum $\overline{p}$ moving in the $+x$ direction. The probability distribution associated with this wavefunction is constant, and the uncertainty in the position of the free particle is approaching infinity. As a consequence, the uncertainty in p will be equal to

$$\Delta p \geq \frac{\hbar / 2}{\Delta x} \to 0$$

The momentum of the particle is thus very well defined, and as a consequence, its energy is also well defined. This is consistent with the fact that the particle has a single well-defined angular frequency.

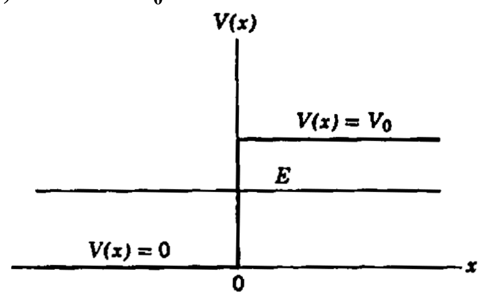
As we have seen in Chapter 3, a realistic particle will be described by a group of waves. The group velocity for each of these waves is equal to

$$v_g = \frac{dE}{dp} = \frac{d}{dp}\left(\frac{p^2}{2m}\right) = \frac{p}{m} = \frac{\hbar}{m}k$$



Each wave will thus propagate with a different velocity. As a result, a free particle that is localized well at time t = 0, will become less localized at a later time since the waves that contribute to its wavefunction propagate with different velocities. This is shown schematically in the Figure on the right where the sum of 200 waves with wave numbers between k = 19 and k = 21 is displayed. The particle is travelling towards the right and the width of the peak increases with increasing time, indicating that the spread in x of the particle increases with time. The Figure was created using the *PsiFreeParticle.nb* Mathematica notebook that can be downloaded from the Physics 237 website.

The Step Potential: $V(x) = 0$ for $x < 0$, $V(x) = V_0$ for $x > 0$, and $E < V_0$.



Consider a particle approaching a step potential with an energy $E < V_0$ (see Figure on the right). When we consider the motion of this particle in a classical model we expect that when the particle approaches the step from the left, the particle will be reflected. It will reverse its direction of motion but the magnitude of its momentum will remain the same ($p = \sqrt{(2mE)}$).

The Schrödinger equation for this system can be written as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad x < 0$$
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -\left(V_0 - E\right)\psi \quad x > 0$$

In the region $x < 0$, the general solution to the Schrödinger equation can be written in the following way:

$$\psi_{x<0}\left(x\right) = Ae^{ik_1x} + Be^{-ik_1x} \quad \text{where} \quad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

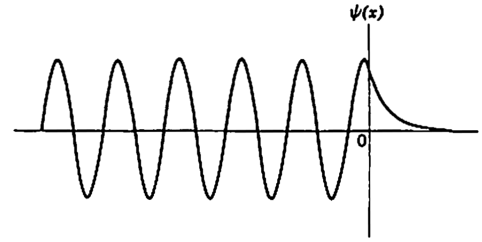
The first term on the right-hand side of the solution describes a wave moving towards the right (**the incident wave**) while the second terms describes a wave moving to the left (**the reflected wave**).

In the region $x > 0$, the general solution to the Schrödinger equation can be written in the following way:

$$\psi_{x>0}\left(x\right) = Ce^{k_2x} + De^{-k_2x} \quad \text{where} \quad k_2 = \frac{\sqrt{2m\left(V_0 - E\right)}}{\hbar}$$

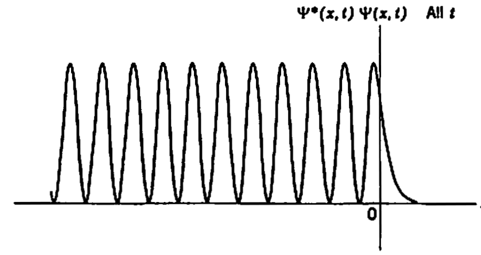
In order for the solutions we indicated above to be valid eigenfunctions, we need to apply the following boundary conditions:

1. **The wavefunctions must be finite for all *x*.** For $x > 0$, this condition requires that $C = 0$ and the wavefunction in this region is thus equal to



$$\psi_{x>0}(x) = De^{-k_2 x} \quad \text{where} \quad k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

2. **The wavefunctions must match at *x* = 0** (see Figure on the right). This requires that



$$\psi_{x<0}(0) = \psi_{x>0}(0) \quad \Rightarrow \quad A + B = D$$

3. **The derivative of the wavefunctions must match at *x* = 0** (see Figure on the right). This requires that

$$\frac{d\psi_{x<0}}{dx}(0) = \frac{d\psi_{x>0}}{dx}(0) \quad \Rightarrow \quad ik_1(A - B) = -k_2 D$$

The last two conditions can be used to obtain a relation between A and B:

$$\left.\begin{array}{l} A + B = D \\ ik_1(A - B) = -k_2 D \end{array}\right\} \quad \Rightarrow \quad ik_1(A - B) = A + B \quad \Rightarrow \quad A = -\left(\frac{k_2 - ik_1}{k_2 + ik_1}\right)B = -\left(\frac{k_2^2 - k_1^2 - 2ik_1k_2}{k_2^2 + k_1^2}\right)B$$

The constant D can now be expressed in terms of the constant B:

$$D = A + B = -\left(\frac{k_2 - ik_1}{k_2 + ik_1}\right)B + B = \frac{(k_2 + ik_1) - (k_2 - ik_1)}{k_2 + ik_1}B = \frac{2ik_1}{k_2 + ik_1}B$$

The **reflection coefficient *R*** is defined as the ratio of the probability density of the reflected wave and the probability density of the incident wave. For the step potential, the reflection coefficient is equal to

$$R = \frac{B^*B}{A^*A} = \frac{B^*B}{\left(\frac{k_2^2 - k_1^2 - 2ik_1k_2}{k_2^2 + k_1^2}\right)^* B^* \left(\frac{k_2^2 - k_1^2 - 2ik_1k_2}{k_2^2 + k_1^2}\right)B} = \frac{\left(k_2^2 + k_1^2\right)^2}{\left(k_2^2 - k_1^2 - 2ik_1k_2\right)\left(k_2^2 - k_1^2 + 2ik_1k_2\right)} = 1$$

The probability of a particle to be reflected is thus equal to 1. However, we should note that the probability density distribution is not equal to zero in the region for which $x > 0$. There is thus a finite probability that the particle penetrates into the classically forbidden region before being reflected. The probability density distribution in this region is equal to

$$P(x) = \psi^*_{x>0}(x)\psi_{x>0}(x) = D^* D e^{-2k_2 x} = \frac{4k_1^2}{k_1^2 + k_2^2} B^* B e^{-2k_2 x}$$

The probability density distribution falls off exponentially with position. The reduction of the probability density distribution is often specified in terms of the distance Δx over which the probability density decreases by $1/e^2$. For the step potential this distance can be obtained by solving the following equation:

$$-2k_2 \Delta x = -2 \quad \Rightarrow \quad \Delta x = \frac{1}{k_2} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

According to the uncertainty principle, this uncertainty in position corresponds to an uncertainty in momentum that satisfies the following relation:

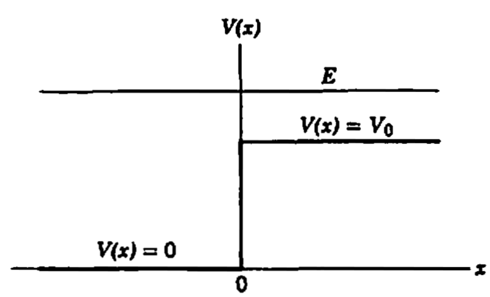
$$\Delta p \geq \frac{\hbar}{\Delta x} = \frac{\hbar}{\left(\dfrac{\hbar}{\sqrt{2m(V_0 - E)}}\right)} = \sqrt{2m(V_0 - E)}$$

The uncertainty in the energy of the particle is thus equal to

$$\Delta E \geq \frac{(\Delta p)^2}{2m} = \frac{1}{2m}\left(2m(V_0 - E)\right) = (V_0 - E)$$

The Step Potential: $V(x) = 0$ for $x < 0$, $V(x) = V_0$ for $x > 0$, and $E > V_0$.

Consider a particle approaching a step potential with an energy $E > V_0$ (see Figure on the right). When we consider the motion of this particle in a classical model we expect that if the particle approaches the step from the left, it will continue to move to the right after passing the step. However, the magnitude of its momentum will be reduced. Classically we expect the following values for the linear momenta in the two regions:



$$p_{x<0} = \sqrt{2mE} \qquad x<0$$
$$p_{x>0} = \sqrt{2m\left(E-V_0\right)} \qquad x>0$$

The Schrödinger equation for this system can be written as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad x<0$$
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \left(E-V_0\right)\psi \qquad x>0$$

In the region $x<0$, the solution to the Schrödinger equation can be written in the following way:

$$\psi_{x<0}\left(x\right) = Ae^{ik_1 x} + Be^{-ik_1 x} \quad \text{where} \quad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

The first term on the right-hand side of the solution describes a wave moving towards the right (the incident wave) while the second terms describes a wave moving to the left (the reflected wave).

In the region $x>0$, the solution to the Schrödinger equation can be written in the following way:

$$\psi_{x>0}\left(x\right) = Ce^{ik_2 x} + De^{-ik_2 x} \quad \text{where} \quad k_2 = \frac{\sqrt{2m\left(E-V_0\right)}}{\hbar}$$

In order for the solutions we indicated above to be valid eigenfunctions, we need to apply the following boundary conditions:

1. **The wavefunction for $x > 0$ is expected to be a wave that moves toward the right**. This condition requires that $D = 0$ and the wavefunction in this region is thus equal to

$$\psi_{x>0}\left(x\right) = Ce^{ik_2 x}$$

2. **The wavefunctions must match at $x = 0$**. This requires that

$$\psi_{x<0}\left(0\right) = \psi_{x>0}\left(0\right) \quad \Rightarrow \quad A+B=C$$

3. **The derivative of the wavefunctions must match at $x = 0$**. This requires that

$$\frac{d\psi_{x<0}}{dx}(0) = \frac{d\psi_{x>0}}{dx}(0) \quad \Rightarrow \quad ik_1(A-B) = ik_2 C$$

The last two conditions can be used to obtain a relation between *A* and *B*:

$$\left.\begin{array}{l} A+B=C \\ ik_1(A-B) = ik_2 C \end{array}\right\} \quad \Rightarrow \quad ik_1(A-B) = ik_2(A+B) \quad \Rightarrow \quad B = \left(\frac{ik_1 - ik_2}{ik_1 + ik_2}\right)A = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)A$$

The constant *C* can now be expressed in terms of the constant *B*:

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

The wavefunction of the particle is thus equal to

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + \left(\dfrac{k_1 - k_2}{k_1 + k_2}\right)Ae^{-ik_1 x} & x < 0 \\ \left(\dfrac{2k_1}{k_1 + k_2}\right)Ae^{ik_2 x} & x > 0 \end{cases}$$

The **reflection coefficient *R*** is defined as the ratio of the probability density of the reflected wave and the probability density of the incident wave. For the step potential, the reflection coefficient is equal to

$$R = \frac{B^* B}{A^* A} = \frac{\left(\dfrac{k_1 - k_2}{k_1 + k_2}\right)A^* \left(\dfrac{k_1 - k_2}{k_1 + k_2}\right)A}{A^* A} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} < 1$$

The probability of a particle to be reflected is thus less than 1. Note that the reflection coefficient is 0 when $k_1 = k_2$. This happens when $V_0 = 0$ (no step) and is thus not a surprise.
The **transmission coefficient *T*** is equal to $1 - R$:

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

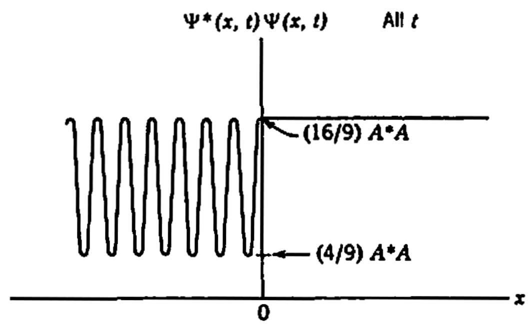
Now consider the probability density distribution in the region for which $x > 0$. The probability density distribution in this region is equal to

$$P(x)=\psi^*_{x>0}(x)\psi_{x>0}(x)=\left(\frac{2k_1}{k_1+k_2}\right)A^*e^{-ik_2x}\left(\frac{2k_1}{k_1+k_2}\right)Ae^{ik_2x}=\left(\frac{2k_1}{k_1+k_2}\right)^2A^*A$$

The probability density distribution in this region is thus constant. The probability density distribution in the $x < 0$ region is equal to

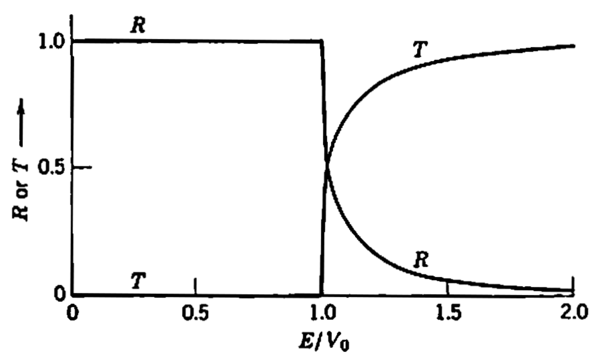
$$\begin{aligned}P(x)\quad &=\psi^*_{x<0}(x)\psi_{x<0}(x)=A^*A\left\{e^{ik_1x}+\frac{k_1-k_2}{k_1+k_2}e^{-ik_1x}\right\}^*\left\{e^{ik_1x}+\frac{k_1-k_2}{k_1+k_2}e^{-ik_1x}\right\}=\\ &=A^*A\left\{e^{-ik_1x}+\frac{k_1-k_2}{k_1+k_2}e^{ik_1x}\right\}\left\{e^{ik_1x}+\frac{k_1-k_2}{k_1+k_2}e^{-ik_1x}\right\}=\\ &=A^*A\left\{1+\left(\frac{k_1-k_2}{k_1+k_2}\right)^2+\frac{k_1-k_2}{k_1+k_2}\left(e^{i2k_1x}+e^{-i2k_1x}\right)\right\}=\\ &=A^*A\left\{1+\left(\frac{k_1-k_2}{k_1+k_2}\right)^2+2\frac{k_1-k_2}{k_1+k_2}\cos(2k_1x)\right\}\end{aligned}$$

An example of the probability density distribution associated with the step potential is shown in the Figure on the right. At $x > 0$, the probability density distribution is constant while at $x < 0$ the probability density distribution is equal to a constant and an oscillatory term.



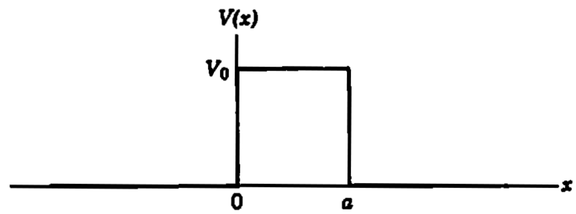
When we repeat the calculation for a particle approaching the step from the right-hand side, we obtain the same reflection and transmission coefficients. We thus conclude that we get reflection anytime the particle encounters a step in the potential; it does not matter if we step up or step down.

We can combine the results of our study of the step potential in the Figure shown on the right. When E is less than the barrier ($E/V_0 < 1$) we saw that there is no transmission ($T = 0$) and only reflection ($R = 1$). When E is larger than the barrier ($E/V_0 > 1$) both reflection and



transmission occur. The transmission coefficient increases with increasing energy above the barrier.

The Potential Barrier: $V(x) = 0$ ($x < 0$), $V(x) = V_0$ ($0 < x < a$), $V(x) = 0$ ($x > a$)



Consider the potential barrier shown in the Figure on the right. We will look at solutions of the Schrödinger equation that are associated with a particle approaching the barrier from the left with an energy $E < V_0$. The solutions in the regions $x < 0$ and $x > a$ are solutions for free particles. In the region $x < 0$ we expect to see the sum of two wave functions: one travelling towards the right (the incident wave) and one travelling towards the left (the reflected wave). In the region $x > 0$ we only expect to see one wave function: one travelling towards the right (the transmitted wave). The most general solution for this problem is given by

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x < 0 \qquad k_1 = \dfrac{\sqrt{2mE}}{\hbar} \\ Fe^{-k_2x} + Ge^{k_2x} & 0 < x < a \qquad k_2 = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar} \\ Ce^{ik_1x} + De^{-ik_1x} & a < x \qquad k_1 = \dfrac{\sqrt{2mE}}{\hbar} \end{cases}$$

Since we do not expect to see waves travelling to the left in the region $x > a$ we must require that $D = 0$. All other constants are not equal to 0. We now can apply the matching conditions:

1. **The wavefunctions must match at $x = 0$**. This requires that

$$\psi_{x<0}(0) = \psi_{x>0}(0) \quad \Rightarrow \quad A + B = F + G$$

2. **The derivative of the wavefunctions must match at $x = 0$**. This requires that

$$\frac{d\psi_{x<0}}{dx}(0) = \frac{d\psi_{x>0}}{dx}(0) \quad \Rightarrow \quad ik_1(A - B) = -k_2(F - G)$$

3. **The wavefunctions must match at $x = a$**. This requires that

$$\psi_{x<a}(a) = \psi_{x>a}(a) \quad \Rightarrow \quad Fe^{-k_2a} + Ge^{k_2a} = Ce^{ik_1a}$$

4. **The derivative of the wavefunctions must match at *x* = *a*.** This requires that

$$\frac{d\psi_{x<a}}{dx}(a) = \frac{d\psi_{x>a}}{dx}(a) \quad \Rightarrow \quad -k_2\left(Fe^{-k_2 a} - Ge^{k_2 a}\right) = ik_1 Ce^{ik_1 a}$$

The reflection and transmission coefficients depend on A, B, and C. The first step will thus be to eliminate F and G. Consider the matching conditions at $x = 0$:

$$\begin{aligned} &A + B = F + G && (1) \\ &A - B = i\frac{k_2}{k_1}(F - G) && (2) \end{aligned}$$

$$\begin{aligned} &(1)+(2): \quad 2A = F\left(1 + i\frac{k_2}{k_1}\right) + G\left(1 - i\frac{k_2}{k_1}\right) \\ &(1)-(2): \quad 2B = F\left(1 - i\frac{k_2}{k_1}\right) + G\left(1 + i\frac{k_2}{k_1}\right) \end{aligned}$$

The matching conditions at $x = a$ can be used to express F and G in terms of C:

$$\begin{aligned} &Fe^{-2k_2 a} + G = Ce^{ik_1 a}e^{-k_2 a} && (1) \\ &Fe^{-2k_2 a} - G = -i\frac{k_1}{k_2}Ce^{ik_1 a}e^{-k_2 a} && (2) \end{aligned}$$

$$\begin{aligned} &(1)+(2): \quad 2Fe^{-2k_2 a} = C\left(1 - i\frac{k_1}{k_2}\right)e^{ik_1 a}e^{-k_2 a} \quad \Rightarrow \quad 2F = C\left(1 - i\frac{k_1}{k_2}\right)e^{ik_1 a}e^{k_2 a} \\ &(1)-(2): \quad 2G = C\left(1 + i\frac{k_1}{k_2}\right)e^{ik_1 a}e^{-k_2 a} \end{aligned}$$

Using these two expressions for F and G we can obtain the following relation between A and C:

$$\begin{aligned} A &= \frac{1}{2}F\left(1 + i\frac{k_2}{k_1}\right) + \frac{1}{2}G\left(1 - i\frac{k_2}{k_1}\right) = \\ &= \frac{1}{4}C\left(1 - i\frac{k_1}{k_2}\right)e^{ik_1 a}e^{k_2 a}\left(1 + i\frac{k_2}{k_1}\right) + \frac{1}{4}C\left(1 + i\frac{k_1}{k_2}\right)e^{ik_1 a}e^{-k_2 a}\left(1 - i\frac{k_2}{k_1}\right) = \\ &= \frac{1}{4}C\left\{\left(2 - i\left(\frac{k_1}{k_2} - \frac{k_2}{k_1}\right)\right)e^{k_2 a} + \left(2 + i\left(\frac{k_1}{k_2} - \frac{k_2}{k_1}\right)\right)e^{-k_2 a}\right\}e^{ik_1 a} \end{aligned}$$

If we define the constant α as $k_1/k_2 - k_2/k_1$, we can rewrite A as

$$A = \frac{1}{4} C \left\{ (2 - i\alpha) e^{k_2 a} + (2 + i\alpha) e^{-k_2 a} \right\} e^{ik_1 a}$$

The complex conjugate of A is thus equal to

$$A^* = \frac{1}{4} C^* \left\{ (2 + i\alpha) e^{k_2 a} + (2 - i\alpha) e^{-k_2 a} \right\} e^{-ik_1 a}$$

The product of A and the complex conjugate of A is equal to

$$\begin{aligned}
A^* A \quad &= \frac{1}{16} C^* C \left\{ (2 + i\alpha) e^{k_2 a} + (2 - i\alpha) e^{-k_2 a} \right\} \left\{ (2 - i\alpha) e^{k_2 a} + (2 + i\alpha) e^{-k_2 a} \right\} = \\
&= \frac{1}{16} C^* C \left\{ \left(4 + \alpha^2\right) \left(e^{k_2 a} + e^{-k_2 a} \right) + (2 - i\alpha)^2 + (2 + i\alpha)^2 \right\} = \\
&= \frac{1}{16} C^* C \left\{ \left(4 + \alpha^2\right) \left(e^{2k_2 a} + e^{-2k_2 a} \right) + \left(4 - 4i\alpha - \alpha^2\right) + \left(4 + 4i\alpha - \alpha^2\right) \right\} = \\
&= \frac{1}{16} C^* C \left\{ \left(4 + \alpha^2\right) \left(e^{2k_2 a} + e^{-2k_2 a} \right) + 2\left(4 - \alpha^2\right) \right\} = \\
&= C^* C \left\{ \frac{1}{16} \left(4 + \alpha^2\right) \left(e^{k_2 a} - e^{-k_2 a} \right)^2 + 1 \right\}
\end{aligned}$$

The constant α can be expressed in terms of the properties of the barrier:

$$\alpha = \frac{k_1}{k_2} - \frac{k_2}{k_1} = \frac{k_1^2 - k_2^2}{k_1 k_2} = \frac{\dfrac{2mE}{\hbar^2} - \dfrac{2m(V_0 - E)}{\hbar^2}}{\dfrac{2m\sqrt{E(V_0 - E)}}{\hbar^2}} = \frac{E - (V_0 - E)}{\sqrt{E(V_0 - E)}} = \frac{2E - V_0}{\sqrt{E(V_0 - E)}}$$

The term $4 + \alpha^2$ can be rewritten as

$$4 + \alpha^2 = 4 + \left(\frac{2E - V_0}{\sqrt{E(V_0 - E)}} \right)^2 = \frac{4E(V_0 - E) + (2E - V_0)^2}{E(V_0 - E)} = \frac{V_0^2}{E(V_0 - E)} = \frac{1}{\dfrac{E}{V_0}\left(1 - \dfrac{E}{V_0}\right)}$$

We can now rewrite the product of the complex conjugate of A and A as

$$A^*A = C^*C\left(1 + \frac{\left(e^{k_2 a} - e^{-k_2 a}\right)^2}{16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)}\right)$$

The transmission coefficient is thus equal to

$$T = \frac{C^*C}{A^*A} = \left(1 + \frac{\left(e^{k_2 a} - e^{-k_2 a}\right)^2}{16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)}\right)^{-1}$$

If $k_2 a >> 1$, we can approximate this expression by

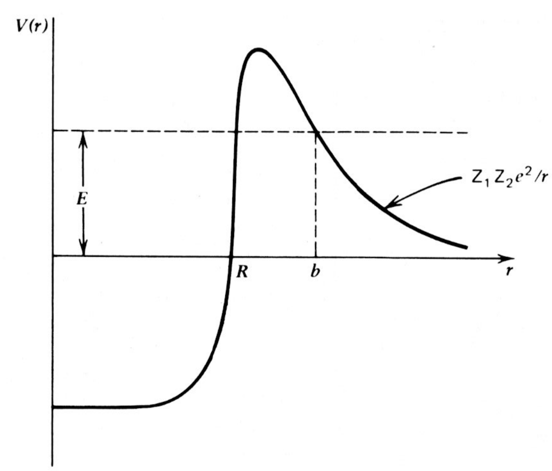
$$T = \frac{C^*C}{A^*A} = \left(1 + \frac{e^{2k_2 a} - 2 + e^{-2k_2 a}}{16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)}\right)^{-1} \underset{k_2 a \gg 1}{=} \left(\frac{e^{2k_2 a}}{16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)}\right)^{-1} = 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2k_2 a}$$

The transmission coefficient depends on the area under the barrier:

$$k_2 a = \sqrt{\frac{2m}{\hbar^2}\left(V_0 - E\right)}a$$

The energy dependence of T is dominated by the energy dependence of the exponential term. When the barrier is position dependent, the exponential term is approximated by

$$e^{-2k_2 a} \to e^{-2\int dx\sqrt{\frac{2m}{\hbar^2}\left(V(x) - E\right)}}$$



Applications of Tunneling

1. Alpha decay.

   Consider the potential that is seen by the alpha particle when it leaves the nucleus. The shape of the potential barrier at $r > R$ is dominated by the repulsive Coulomb potential. At distances $r < R$ the potential is dominated by the strong attractive nuclear potential. Assume that the energy of the alpha particle is E. The transmission probability is proportional to

$$T \simeq e^{-2\int_R^b \sqrt{\frac{2m}{\hbar^2}(V(r)-E)}\,dr} = e^{-2\sqrt{\frac{2m}{\hbar^2}}\int_R^b \sqrt{\left(\frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r}-E\right)}\,dr}$$

where Z_1 is the charge of the daughter nucleus (the charge of the nucleus after alpha emission) and Z_2 is the charge of the alpha particle ($Z_2 = 2$). The turning point b is defined as the point where the alpha particle emerges from the barrier. At this position, the Coulomb potential is equal to the energy of the alpha particle:

$$E = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{b}$$

The integral can be evaluated exactly:

$$\int_R^b \sqrt{\left(\frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r}-E\right)}\,dr = \int_R^b \sqrt{\left(\frac{1}{4\pi\varepsilon_0}\left(\frac{Z_1 Z_2 e^2}{r}-\frac{Z_1 Z_2 e^2}{b}\right)\right)}\,dr =$$

$$= \sqrt{\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0}}\sqrt{b}\left\{\cos^{-1}\left(\sqrt{\frac{R}{b}}\right)-\sqrt{\frac{R}{b}-\frac{R^2}{b^2}}\right\}$$

At low energies, low compared to the height of the barrier, $b >> R$ and the integral is approximately equal to

$$\int_R^b \sqrt{\left(\frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r}-E\right)}\,dr \underset{b>>R}{=} \sqrt{\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0}}\sqrt{b}\left\{\frac{\pi}{2}-\sqrt{\frac{R}{b}}\right\}$$

This expression can be rewritten as

$$\int_R^b \sqrt{\left(\frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r}-E\right)}\,dr \approx \sqrt{\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0}}\sqrt{b}\left(\frac{\pi}{2}\right) = \sqrt{\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0}}\sqrt{\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 E}}\left(\frac{\pi}{2}\right) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0}\left(\frac{\pi}{2}\right)\frac{1}{\sqrt{E}}$$

The exponent is thus equal to

$$2\sqrt{\frac{2m}{\hbar^2}}\int_R^b \sqrt{\left(\frac{1}{4\pi\varepsilon_0}\frac{Z_1Z_2e^2}{r}-E\right)}dr \quad = 2\sqrt{\frac{2m}{\hbar^2}}\frac{Z_1Z_2e^2}{4\pi\varepsilon_0}\frac{\pi}{2}\frac{1}{\sqrt{E}} = 2\sqrt{\frac{2mc^2}{\hbar^2c^2}}\frac{e^2}{4\pi\varepsilon_0}\pi\frac{Z_1}{\sqrt{E}} =$$

$$= 2\pi\sqrt{2mc^2}\frac{e^2}{4\pi\varepsilon_0\hbar c}\left(\frac{Z_1}{\sqrt{E}}\right) \simeq 562\frac{1}{137}\left(\frac{Z_1}{\sqrt{E}}\right) = 4\left(\frac{Z_1}{\sqrt{E}}\right)$$

where E is the energy of the alpha particle in MeV. The probability that the alpha particle tunnels through the barrier is thus equal to

$$T \approx e^{-4\left(\frac{Z_1}{\sqrt{E}}\right)}$$

In order for the alpha particle to tunnel through the barrier, it must interact with the barrier n times where

$$n \approx e^{4\left(\frac{Z_1}{\sqrt{E}}\right)}$$

In a very classical picture, we can assume that if the alpha particle is reflected, it will encounter the barrier again on the other side of the nucleus. The number of collisions of the alpha particle with the barrier per second is equal to

$$r_{collisions} = \frac{v}{2R}$$

where v is the velocity of the alpha particle. The typical energy of alpha particles produced in nuclear decays is 1 – 10 MeV. The velocity of a 1 MeV alpha particle is equal to

$$v = \sqrt{\frac{2E}{m}} = c\sqrt{\frac{2E}{mc^2}} \approx c\sqrt{\frac{2\times 1}{4000}} = c\sqrt{\frac{1}{2000}} = 6.7\times 10^6 \text{ m/s}$$

The velocity of a 10 MeV alpha particle is 2.1×10^7 m/s. The radius of a nucleus of 1.5 $A^{1/3}$ fm. For A = 200, we find R = 8.7 fm. The collision rate for a 1 MeV alpha particle is thus equal to

$$r_{collisions} = \frac{6.7\times 10^6}{2\left(8.7\times 10^{-15}\right)} = 2.3\times 10^{20} \text{ s}^{-1}$$

The lifetime of the nucleus is thus equal to

$$\tau = \frac{n}{r_{collisions}} \approx \frac{2R}{v} e^{4\left(\frac{Z_1}{\sqrt{E}}\right)}$$

It is customary to look at the relation between the decay rate $1/\tau$ and the energy of the alpha particle:

$$\frac{1}{\tau} \approx \frac{v}{2R} e^{-4\left(\frac{Z_1}{\sqrt{E}}\right)} \quad \Rightarrow \quad \log\frac{1}{\tau} = \log\frac{v}{2R} - 1.7\frac{Z_1}{\sqrt{E}} \approx 20 - 1.7\frac{Z_1}{\sqrt{E}}$$

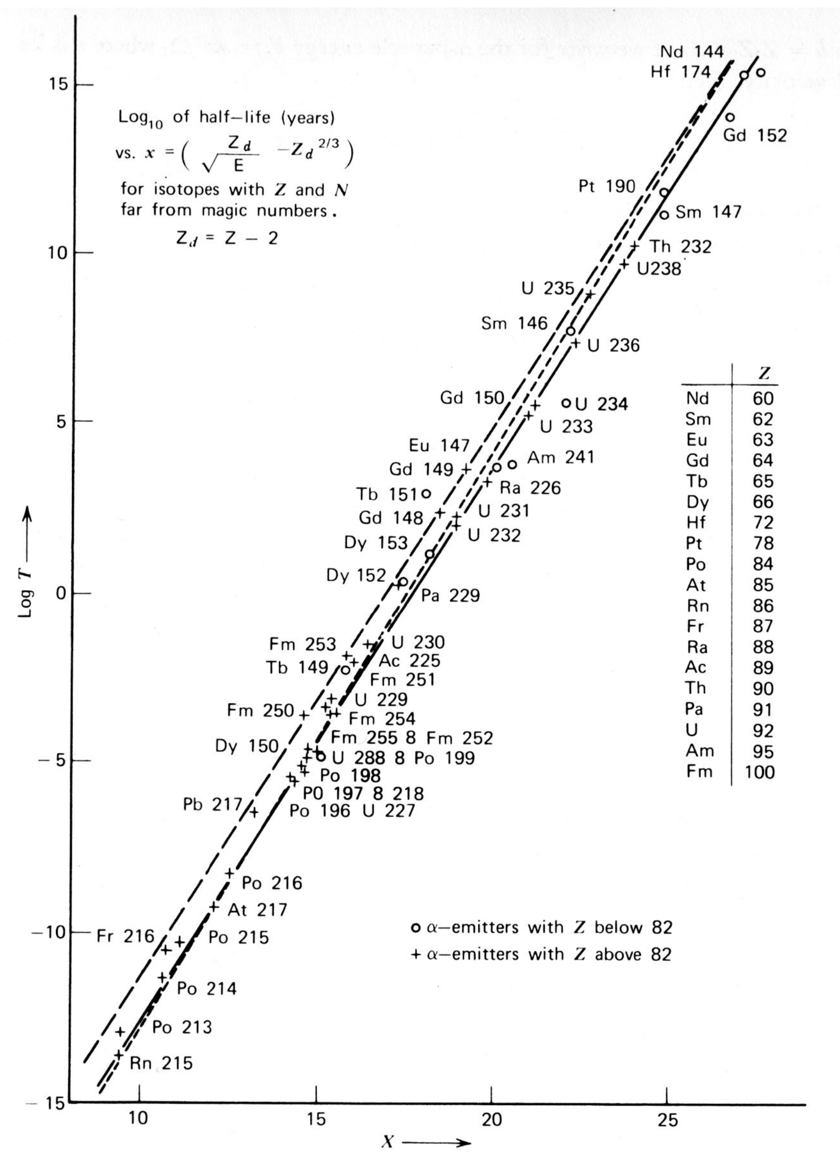
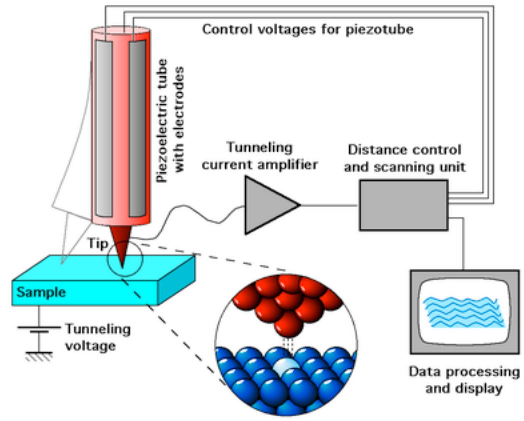


Fig. 5-13. Plot of $\log_{10} 1/\tau$ versus $C_2 - C_1 Z_1/\sqrt{E}$ with $C_1 = 1.61$ and a slowly varying $C_2 = 28.9 + 1.6\, Z_1^{2/3}$. (From E. K. Hyde, I. Perlman and G. T. Seaborg, *The Nuclear Properties of the Heavy Elements*, Vol. 1, Prentice-Hall, Inc. (1964), reprinted by permission.)

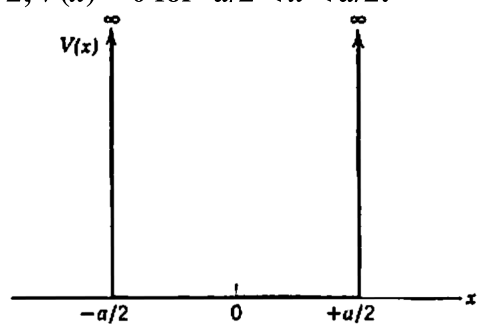
2. **Scanning Tunneling Microscope**



The scanning tunneling microscope relies on the exponential dependence of the transmission coefficient on the barrier width. Small variations in a lead to huge variations in T.

A schematic of the operation of the scanning tunneling microscope is shown in the Figure on the right, obtained from http://www.absoluteastronomy.com/topics/Scanning_tunneling_microscope. An electric current tunnels through the gap between the sample and the tip. The position of the tip is adjusted such that the current stays constant. In this way, the position of the tip follows the structure of the surface; the structure of the surface can thus can be mapped with great precision.

The Infinite Square Well: $V(x) = \infty$ for $x < -a/2$ and $x > a/2$, $V(x) = 0$ for $-a/2 < x < a/2$.



Since the potential in the region $x < -a/2$ and $x > a/2$ is infinite, the probability to find a particle in these regions is zero. The wavefunction in this region is thus also 0. In the region $-a/2 < x < a/2$, the wavefunction should have the same form as the wavefunction of the free particle. We thus conclude that

$$\psi(x) = \begin{cases} 0 & x < -\dfrac{a}{2} \\ Ae^{ikx} + Be^{-ikx} & -\dfrac{a}{2} < x < \dfrac{a}{2} \\ 0 & \dfrac{a}{2} < x \end{cases}$$

We note that the solutions inside the well can be written as the sum of a cosine and sine function:

$$\begin{aligned} Ae^{ikx} + Be^{-ikx} &= \left(\frac{B'}{2} + \frac{A'}{2i}\right)e^{ikx} + \left(\frac{B'}{2} - \frac{A'}{2i}\right)e^{-ikx} = \\ &= B'\left(\frac{e^{ikx} + e^{-ikx}}{2}\right) + A'\left(\frac{e^{ikx} - e^{-ikx}}{2i}\right) = B'\cos(kx) + A'\sin(kx) \end{aligned}$$

The following boundary conditions are required to be satisfied:

1. **The wavefunction must be continuous at *x* = -*a*/2 and at *x* = *a*/2**. This requires that:

$$\psi\left(x=-\frac{a}{2}\right)=B'\cos\left(-k\frac{a}{2}\right)+A'\sin\left(-k\frac{a}{2}\right)=B'\cos\left(k\frac{a}{2}\right)-A'\sin\left(k\frac{a}{2}\right)=0 \quad (1)$$

$$\psi\left(x=+\frac{a}{2}\right)=B'\cos\left(k\frac{a}{2}\right)+A'\sin\left(k\frac{a}{2}\right)=0 \quad (2)$$

2. **Since the potential goes to infinity at *x* = -*a*/2 and at *x* = *a*/2 there is no requirement that the slope of the wavefunction is continuous at *x* = -*a*/2 and at *x* = *a*/2**.

By manipulating the equations that are consistent with condition 1 we can conclude:

$$(1)+(2)=2B'\cos\left(k\frac{a}{2}\right)=0 \quad\Rightarrow\quad k\frac{a}{2}=\frac{\pi}{2},\frac{3\pi}{2},\frac{5\pi}{2},\ldots \quad\Rightarrow\quad k=\frac{\pi}{a},\frac{3\pi}{a},\frac{5\pi}{a},\ldots$$

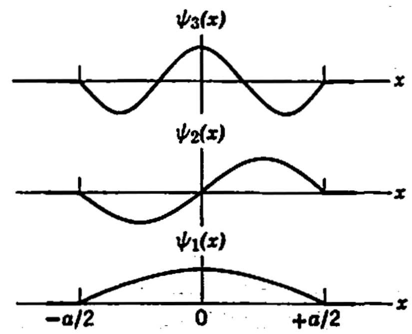
$$(1)-(2)=2A'\sin\left(k\frac{a}{2}\right)=0 \quad\Rightarrow\quad k\frac{a}{2}=\pi,2\pi,3\pi,\ldots \quad\Rightarrow\quad k=\frac{2\pi}{a},\frac{4\pi}{a},\frac{\pi}{a},\ldots$$

Both of these conditions must be satisfied at the same time. Consider the following 2 possibilities:

1. If $B'\neq 0 \quad\Rightarrow\quad \cos\left(k\frac{a}{2}\right)=0 \quad\Rightarrow\quad \sin\left(k\frac{a}{2}\right)=\pm 1 \quad\Rightarrow\quad A'=0$
2. If $A'\neq 0 \quad\Rightarrow\quad \sin\left(k\frac{a}{2}\right)=0 \quad\Rightarrow\quad \cos\left(k\frac{a}{2}\right)=\pm 1 \quad\Rightarrow\quad B'=0$

The general solution of the infinite square well can thus be written as:

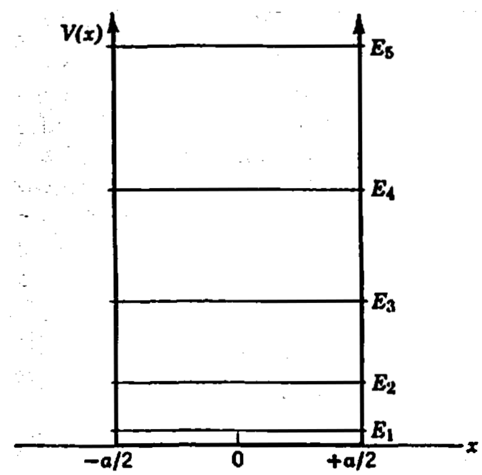
$$\psi(x)=\begin{cases} 0 & x<-\frac{a}{2} \\ A_n\sin(k_n x), \quad k_n=\frac{n\pi}{a}, \quad n=2,4,6,\ldots. & \\ & -\frac{a}{2}<x<\frac{a}{2} \\ B_n\cos(k_n x), \quad k_n=\frac{n\pi}{a}, \quad n=1,3,5,\ldots. & \\ 0 & \frac{a}{2}<x \end{cases}$$



Examples of the wavefunctions for n = 1, 2, and 3 are shown in the Figure on the right. We observe that for odd n the wavefunction is even (**even parity**) while for even n the wavefunction is odd (**odd parity**).

The value of k_n is quantized. Since k_n is related to the energy of the particle, the energy is also quantized:

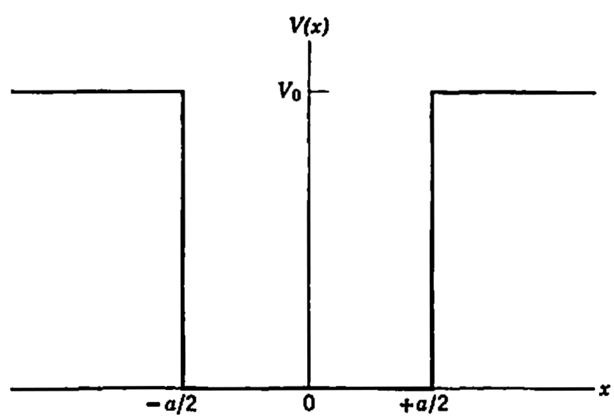
$$k_n = \frac{n\pi}{a} = \frac{\sqrt{2mE_n}}{\hbar} \quad \Rightarrow \quad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2\hbar^2 n^2}{2m}, \quad n = 1,2,3,....$$



The energy of the particle is thus never equal to 0. The lowest 5 energy levels for the infinite well are schematically shown in the Figure on the right. The spacing between individual levels increases when n increases.

The Finite Square Well: $V(x) = V_0$ for $x < -a/2$ and $x > a/2$, $V(x) = 0$ for $-a/2 < x < a/2$.

The infinite square well shows how quantization of energy emerges from the Schrödinger equation. However, it is not realistic to assume that the potential approaches infinity in regions outside the well, and a more realistic study of a potential well requires us to consider the finite square well.



The finite square well is shown schematically in the Figure on the right. Assuming that the energy of the particle we are describing is below V_0 we expect to see exponentially decaying wavefunctions in the regions where $x < -a/2$ or $x > a/2$. Inside the well, the shape of the wavefunctions should be similar to the shape of the wavefunctions in this region for the infinite well, except that the value of the wavefunction at the walls is no longer required to be zero.

The most general solution of the Schrödinger equation for this potential is given by the following expression:

$$\psi(x)=\begin{cases} Ce^{k_2 x}+De^{-k_2 x} & \text{where } k_2=\dfrac{\sqrt{2m(V_0-E)}}{\hbar} \quad x<-\dfrac{a}{2} \\ A\sin(k_1 x)+B\cos(k_1 x) & \text{where } k_1=\dfrac{\sqrt{2mE}}{\hbar} \quad -\dfrac{a}{2}<x<\dfrac{a}{2} \\ Fe^{k_2 x}+Ge^{-k_2 x} & \text{where } k_2=\dfrac{\sqrt{2m(V_0-E)}}{\hbar} \quad \dfrac{a}{2}<x \end{cases}$$

In order for this wavefunction to be a valid eigenfunction we must require that the following conditions are met:

1. **Require that the eigenfunction remains finite**. In order to ensure that this requirement is met when x approach ± infinity we must require that $D = F = 0$.

2. **The wavefunctions must match at *x* = -*a*/2**. This requires that

$$\psi\left(x\uparrow -\frac{a}{2}\right)=\psi\left(x\downarrow -\frac{a}{2}\right) \quad\Rightarrow\quad Ce^{-k_2\frac{a}{2}}=A\sin\left(-k_1\frac{a}{2}\right)+B\cos\left(-k_1\frac{a}{2}\right)$$

3. **The derivative of the wavefunctions must match at *x* = -*a*/2**. This requires that

$$\frac{d\psi}{dx}\left(x\uparrow -\frac{a}{2}\right)=\frac{d\psi}{dx}\left(x\downarrow -\frac{a}{2}\right) \quad\Rightarrow\quad Ck_2e^{-k_2\frac{a}{2}}=Ak_1\cos\left(-k_1\frac{a}{2}\right)-Bk_1\sin\left(-k_1\frac{a}{2}\right)$$

4. **The wavefunctions must match at *x* = *a*/2**. This requires that

$$\psi\left(x\downarrow \frac{a}{2}\right)=\psi\left(x\uparrow \frac{a}{2}\right) \quad\Rightarrow\quad Ge^{-k_2\frac{a}{2}}=A\sin\left(k_1\frac{a}{2}\right)+B\cos\left(k_1\frac{a}{2}\right)$$

5. **The derivative of the wavefunctions must match at *x* = *a*/2**. This requires that

$$\frac{d\psi}{dx}\left(x\downarrow -\frac{a}{2}\right)=\frac{d\psi}{dx}\left(x\uparrow -\frac{a}{2}\right) \quad\Rightarrow\quad -Gk_2e^{-k_2\frac{a}{2}}=Ak_1\cos\left(k_1\frac{a}{2}\right)-Bk_1\sin\left(k_1\frac{a}{2}\right)$$

The total number of unknown in these fours equations is 5: A, B, C, G, and the energy E, which defines k_1 and k_2. It would appear that we cannot uniquely determine the unknown. But we should realize that the wavefunction must be normalized and there is thus one addition requirement that must be satisfied by the wavefunction.

Consider the following 4 requirements obtained from the matching requirements:

$$Ce^{-k_2\frac{a}{2}} = A\sin\left(-k_1\frac{a}{2}\right) + B\cos\left(-k_1\frac{a}{2}\right) = -A\sin\left(k_1\frac{a}{2}\right) + B\cos\left(k_1\frac{a}{2}\right)$$

$$Ck_2e^{-k_2\frac{a}{2}} = Ak_1\cos\left(-k_1\frac{a}{2}\right) - Bk_1\sin\left(-k_1\frac{a}{2}\right) = Ak_1\cos\left(k_1\frac{a}{2}\right) + Bk_1\sin\left(k_1\frac{a}{2}\right)$$

$$Ge^{-k_2\frac{a}{2}} = A\sin\left(k_1\frac{a}{2}\right) + B\cos\left(k_1\frac{a}{2}\right)$$

$$-Gk_2e^{-k_2\frac{a}{2}} = Ak_1\cos\left(k_1\frac{a}{2}\right) - Bk_1\sin\left(k_1\frac{a}{2}\right)$$

We can rewrite these equations in the following way:

$$-A\sin\left(k_1\frac{a}{2}\right) + B\cos\left(k_1\frac{a}{2}\right) - Ce^{-k_2\frac{a}{2}} = 0$$

$$Ak_1\cos\left(k_1\frac{a}{2}\right) + Bk_1\sin\left(k_1\frac{a}{2}\right) - Ck_2e^{-k_2\frac{a}{2}} = 0$$

$$A\sin\left(k_1\frac{a}{2}\right) + B\cos\left(k_1\frac{a}{2}\right) - Ge^{-k_2\frac{a}{2}} = 0$$

$$Ak_1\cos\left(k_1\frac{a}{2}\right) - Bk_1\sin\left(k_1\frac{a}{2}\right) + Gk_2e^{-k_2\frac{a}{2}} = 0$$

or

$$\begin{pmatrix} -\sin\left(k_1\frac{a}{2}\right) & \cos\left(k_1\frac{a}{2}\right) & -e^{-k_2\frac{a}{2}} & 0 \\ k_1\cos\left(k_1\frac{a}{2}\right) & k_1\sin\left(k_1\frac{a}{2}\right) & -k_2e^{-k_2\frac{a}{2}} & 0 \\ \sin\left(k_1\frac{a}{2}\right) & \cos\left(k_1\frac{a}{2}\right) & 0 & -e^{-k_2\frac{a}{2}} \\ k_1\cos\left(k_1\frac{a}{2}\right) & -k_1\sin\left(k_1\frac{a}{2}\right) & 0 & k_2e^{-k_2\frac{a}{2}} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ G \end{pmatrix} = 0$$

This equation has a non-trivial solution when the determinant of the matrix vanishes. This requires that

$$\begin{vmatrix} -\sin\left(k_1 \frac{a}{2}\right) & \cos\left(k_1 \frac{a}{2}\right) & -e^{-k_2 \frac{a}{2}} & 0 \\ k_1 \cos\left(k_1 \frac{a}{2}\right) & k_1 \sin\left(k_1 \frac{a}{2}\right) & -k_2 e^{-k_2 \frac{a}{2}} & 0 \\ \sin\left(k_1 \frac{a}{2}\right) & \cos\left(k_1 \frac{a}{2}\right) & 0 & -e^{-k_2 \frac{a}{2}} \\ k_1 \cos\left(k_1 \frac{a}{2}\right) & -k_1 \sin\left(k_1 \frac{a}{2}\right) & 0 & k_2 e^{-k_2 \frac{a}{2}} \end{vmatrix} = 0$$

This is equivalent to

$$-\sin\left(k_1 \frac{a}{2}\right) \begin{vmatrix} k_1 \sin\left(k_1 \frac{a}{2}\right) & -k_2 e^{-k_2 \frac{a}{2}} & 0 \\ \cos\left(k_1 \frac{a}{2}\right) & 0 & -e^{-k_2 \frac{a}{2}} \\ -k_1 \sin\left(k_1 \frac{a}{2}\right) & 0 & k_2 e^{-k_2 \frac{a}{2}} \end{vmatrix} - \cos\left(k_1 \frac{a}{2}\right) \begin{vmatrix} k_1 \cos\left(k_1 \frac{a}{2}\right) & -k_2 e^{-k_2 \frac{a}{2}} & 0 \\ \sin\left(k_1 \frac{a}{2}\right) & 0 & -e^{-k_2 \frac{a}{2}} \\ k_1 \cos\left(k_1 \frac{a}{2}\right) & 0 & k_2 e^{-k_2 \frac{a}{2}} \end{vmatrix}$$

$$- e^{-k_2 \frac{a}{2}} \begin{vmatrix} k_1 \cos\left(k_1 \frac{a}{2}\right) & k_1 \sin\left(k_1 \frac{a}{2}\right) & 0 \\ \sin\left(k_1 \frac{a}{2}\right) & \cos\left(k_1 \frac{a}{2}\right) & -e^{-k_2 \frac{a}{2}} \\ k_1 \cos\left(k_1 \frac{a}{2}\right) & -k_1 \sin\left(k_1 \frac{a}{2}\right) & k_2 e^{-k_2 \frac{a}{2}} \end{vmatrix} = 0$$

Each determinant can be evaluated:

$$\begin{vmatrix} k_1 \sin\left(k_1 \frac{a}{2}\right) & -k_2 e^{-k_2 \frac{a}{2}} & 0 \\ \cos\left(k_1 \frac{a}{2}\right) & 0 & -e^{-k_2 \frac{a}{2}} \\ -k_1 \sin\left(k_1 \frac{a}{2}\right) & 0 & k_2 e^{-k_2 \frac{a}{2}} \end{vmatrix} = k_2 e^{-k_2 a} \left(k_2 \cos\left(k_1 \frac{a}{2}\right) - k_1 \sin\left(k_1 \frac{a}{2}\right) \right)$$

$$\begin{vmatrix} k_1\cos\left(k_1\frac{a}{2}\right) & -k_2 e^{-k_2\frac{a}{2}} & 0 \\ \sin\left(k_1\frac{a}{2}\right) & 0 & -e^{-k_2\frac{a}{2}} \\ k_1\cos\left(k_1\frac{a}{2}\right) & 0 & k_2 e^{-k_2\frac{a}{2}} \end{vmatrix} = k_2 e^{-k_2 a}\left(k_2\sin\left(k_1\frac{a}{2}\right)+k_1\cos\left(k_1\frac{a}{2}\right)\right)$$

$$\begin{vmatrix} k_1\cos\left(k_1\frac{a}{2}\right) & k_1\sin\left(k_1\frac{a}{2}\right) & 0 \\ \sin\left(k_1\frac{a}{2}\right) & \cos\left(k_1\frac{a}{2}\right) & -e^{-k_2\frac{a}{2}} \\ k_1\cos\left(k_1\frac{a}{2}\right) & -k_1\sin\left(k_1\frac{a}{2}\right) & k_2 e^{-k_2\frac{a}{2}} \end{vmatrix} = \begin{array}{l} k_1\cos\left(k_1\frac{a}{2}\right)\left(\cos\left(k_1\frac{a}{2}\right)k_2-k_1\sin\left(k_1\frac{a}{2}\right)\right)e^{-k_2\frac{a}{2}} - \\ k_1\sin\left(k_1\frac{a}{2}\right)\left(\sin\left(k_1\frac{a}{2}\right)k_2+k_1\cos\left(k_1\frac{a}{2}\right)\right)e^{-k_2\frac{a}{2}} = \end{array}$$

$$=\left[k_1k_2\cos^2\left(k_1\frac{a}{2}\right)-2k_1^2\cos\left(k_1\frac{a}{2}\right)\sin\left(k_1\frac{a}{2}\right)-k_1k_2\sin^2\left(k_1\frac{a}{2}\right)\right]e^{-k_2\frac{a}{2}} =$$

$$=k_1k_2\left(\cos^2\left(k_1\frac{a}{2}\right)-\sin^2\left(k_1\frac{a}{2}\right)\right)e^{-k_2\frac{a}{2}}-2k_1^2\cos\left(k_1\frac{a}{2}\right)\sin\left(k_1\frac{a}{2}\right)e^{-k_2\frac{a}{2}}$$

The determinant of the matrix is thus equal to

$$-\sin\left(k_1\frac{a}{2}\right)k_2e^{-k_2a}\left(k_2\cos\left(k_1\frac{a}{2}\right)-k_1\sin\left(k_1\frac{a}{2}\right)\right)-\cos\left(k_1\frac{a}{2}\right)k_2e^{-k_2a}\left(k_2\sin\left(k_1\frac{a}{2}\right)+k_1\cos\left(k_1\frac{a}{2}\right)\right)$$

$$-e^{-k_2a}k_1k_2\left(\cos^2\left(k_1\frac{a}{2}\right)-\sin^2\left(k_1\frac{a}{2}\right)\right)e^{-k_2\frac{a}{2}}-2k_1^2\cos\left(k_1\frac{a}{2}\right)\sin\left(k_1\frac{a}{2}\right)e^{-k_2\frac{a}{2}} \quad =$$

$$=-2\left(k_1^2+k_2^2\right)e^{-k_2a}\sin\left(k_1\frac{a}{2}\right)\cos\left(k_1\frac{a}{2}\right)+2k_1k_2e^{-k_2a}\sin^2\left(k_1\frac{a}{2}\right)-2k_1k_2e^{-k_2a}\cos^2\left(k_1\frac{a}{2}\right)=0$$

This requires that

$$2\left(k_1^2+k_2^2\right)\sin\left(k_1\frac{a}{2}\right)\cos\left(k_1\frac{a}{2}\right)-2k_1k_2\sin^2\left(k_1\frac{a}{2}\right)+2k_1k_2\cos^2\left(k_1\frac{a}{2}\right)=0$$

This equation can be rewritten as

$$\left(k_1^2+k_2^2\right)\sin\left(2k_1\frac{a}{2}\right)+2k_1k_2\cos\left(2k_1\frac{a}{2}\right)=0 \quad \Rightarrow \quad \left(k_1^2+k_2^2\right)+2k_1k_2\cot\left(2k_1\frac{a}{2}\right)=0$$

This equation can be used to express k_2 in terms of k_1:

$$k_2^2 + 2k_1 \cot\left(2k_1 \frac{a}{2}\right) k_2 + k_1^2 = 0 \quad \Rightarrow$$

$$\begin{aligned}
k_2 &= \frac{-2k_1 \cot\left(2k_1 \frac{a}{2}\right) \pm \sqrt{4k_1^2 \cot^2\left(2k_1 \frac{a}{2}\right) - 4k_1^2}}{2} = -k_1 \cot\left(2k_1 \frac{a}{2}\right) \pm k_1 \sqrt{\cot^2\left(2k_1 \frac{a}{2}\right) - 1} = \\
&= -k_1 \frac{\cos^2\left(k_1 \frac{a}{2}\right) - \sin^2\left(k_1 \frac{a}{2}\right)}{2\sin\left(k_1 \frac{a}{2}\right)\cos\left(k_1 \frac{a}{2}\right)} \pm k_1 \sqrt{\frac{\left(\cos^2\left(k_1 \frac{a}{2}\right) - \sin^2\left(k_1 \frac{a}{2}\right)\right)^2}{4\sin^2\left(k_1 \frac{a}{2}\right)\cos^2\left(k_1 \frac{a}{2}\right)} - 1} = \\
&= -k_1 \frac{\cos^2\left(k_1 \frac{a}{2}\right) - \sin^2\left(k_1 \frac{a}{2}\right)}{2\sin\left(k_1 \frac{a}{2}\right)\cos\left(k_1 \frac{a}{2}\right)} \pm k_1 \frac{\cos^2\left(k_1 \frac{a}{2}\right) - \sin^2\left(k_1 \frac{a}{2}\right)}{2\sin\left(k_1 \frac{a}{2}\right)\cos\left(k_1 \frac{a}{2}\right)} = \\
&= \begin{cases} k_1 \dfrac{\sin^2\left(k_1 \frac{a}{2}\right)}{\sin\left(k_1 \frac{a}{2}\right)\cos\left(k_1 \frac{a}{2}\right)} = k_1 \tan\left(k_1 \frac{a}{2}\right) \\[2ex] -k_1 \dfrac{\cos^2\left(k_1 \frac{a}{2}\right)}{\sin\left(k_1 \frac{a}{2}\right)\cos\left(k_1 \frac{a}{2}\right)} = -k_1 \cot\left(k_1 \frac{a}{2}\right) \end{cases}
\end{aligned}$$

The requirement to find a solution is thus equivalent to the following two requirements:

$$k_2 = \begin{cases} k_1 \tan\left(k_1 \frac{a}{2}\right) \\ -k_1 \cot\left(k_1 \frac{a}{2}\right) \end{cases}$$

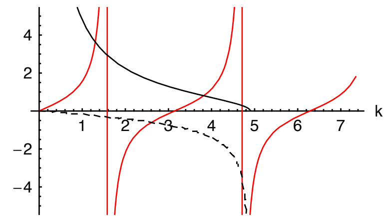
But, k_2 is related to k_1:

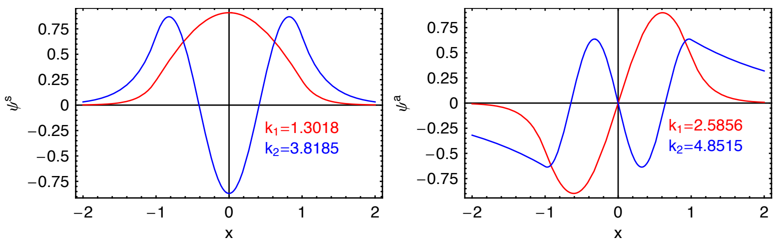
$$k_2^2 = \frac{2m\left(V_0 - E\right)}{\hbar^2} = \frac{2mV_0}{\hbar^2} - \frac{2mE}{\hbar^2} = \frac{2mV_0}{\hbar^2} - k_1^2$$

The requirements to find a solution can thus be rewritten as:

$$\frac{1}{k_1}\sqrt{\frac{2mV_0}{\hbar^2}-k_1^2}=\tan\left(k_1\frac{a}{2}\right) \quad \text{and} \quad -k_1\frac{1}{\sqrt{\frac{2mV_0}{\hbar^2}-k_1^2}}=\tan\left(k_1\frac{a}{2}\right)$$

To find values of $k1$ for which solutions can be found we can examine plots of the left-hand side of each equation and the right-hand side of each equation. An example is shown in the Figure on the right. For this example, there are 4 eigen values. The corresponding eigenfunctions are shown in the Figures below.





The Simple Harmonic Oscillator

One important potential in many areas of physics is the harmonic oscillator. It describes the potential around an equilibrium position for a divers range of systems. When we look in the vicinity of the equilibrium position, we find that many potential distributions have a shape similar to that of the simple harmonic oscillator:

$$V(x)=\frac{1}{2}Cx^2$$

In classical physics, we expect that the motion associated with the harmonic oscillator has a frequency equal to

$$\nu=\frac{1}{2\pi}\sqrt{\frac{C}{m}}$$

According to Planck, the energy associated with the harmonic oscillator is quantized and equal to

$$E_n=nh\nu \qquad n=0,1,2,....$$

When we solve the Schrödinger equation for the simple harmonic oscillator we find the that energy of the solutions can be written as

$$E_n = \left(n + \frac{1}{2} \right) h\nu \qquad n = 0,1,2,....$$

The biggest difference between the classical and the quantum mechanical solution is the zero-point energy. In the classical model, the energy of the system can be zero (n = 0); in the quantum mechanical model, the energy for n = 0 is $h\nu/2$. The limit of E is due to the uncertainty principle.

Consider the classical turning points for n = 0:

$$\frac{1}{2} h\nu = \frac{1}{2} C x^2 \quad \Rightarrow \quad x = \pm \sqrt{\frac{h\nu}{C}}$$

The uncertainty in x is thus equal to

$$\Delta x = \sqrt{\frac{h\nu}{C}}$$

According to the uncertainty principle, the uncertainty in x produces an uncertainty in p:

$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{\hbar}{2} \sqrt{\frac{C}{h\nu}}$$

The corresponding uncertainty in the energy is equal to

$$\Delta E = \Delta \left(\frac{p^2}{2m} \right) = \frac{2p\Delta p}{2m} \geq \frac{\left(\frac{\hbar}{2} \sqrt{\frac{C}{h\nu}} \right)^2}{m} = \frac{\left(\frac{\hbar^2}{4} \frac{C}{h\nu} \right)}{m} = \frac{\left(\frac{\hbar^2}{4} \frac{\left(4\pi^2 \nu^2 m\right)}{h\nu} \right)}{m} = \frac{1}{4} h\nu$$