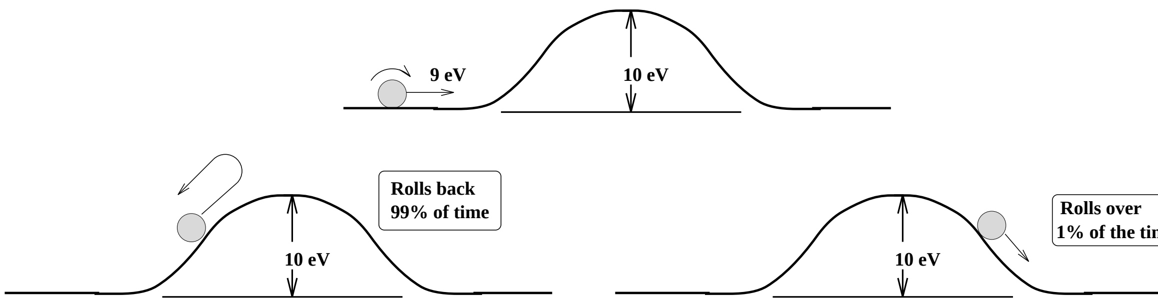
Quantum Tunneling

In this chapter, we discuss the phenomena which allows an electron to quantum tunnel over a classically forbidden barrier.



This is a strikingly non-intuitive process where small changes in either the height or width of a barrier create large changes the tunneling current of particles crossing the barrier. Quantum tunneling controls natural phenomena such as radioactive α decay where a factor of three increase in the energy released during a decay is responsible for a 10^{20} fold increase in the α decay rate. The inherent sensitivity of the tunneling process can be exploited to produce photographs of individual atoms using scanning tunneling microscopes (STM) or produce extremely rapid amplifiers using tunneling diodes. It is an area of physics which is as philosophically fascinating as it is technologically important.

Most of this chapter deals with *continuum* rather than bound state systems. In bound state problems, one is usually concerned with solving for possible stationary state energies. In tunneling problems, one has a continuous spectrum of possible incident energies. In these problems we are generally concerned with solving for the probability that an electron is transmitted or reflected from a given barrier in terms of its known incident energy.

Quantum Current

Tunneling is described by a transmission coefficient which gives the ratio of the current density emerging from a barrier divided by the current density incident on a barrier. Classically the current density $\vec{J}$ is related to the charge density ρ and the velocity charge velocity $\vec{v}$ according to $\vec{J} = \rho\, \vec{v}$. Its natural to relate the current density ρ with the electron charge e and the quantum PDF(x) according to $\rho = e\Psi^*(x)\Psi(x)$. It is equally natural to describe the velocity by $\hat{p}/m$ where (in 3 dimensions) $\check{p} = -i\hbar(\partial/\partial x) \rightarrow -i\hbar\vec{\nabla}$. Of course $\vec{\nabla}$ is an operator which needs to operate on part of ρ. Recalling this same issue from our discussion on **Quantum Measurement** we expect:

$$\vec{J} \sim \frac{e}{m}\Psi^*\vec{\nabla}\Psi \tag{1}$$

This form isn't totally correct but fairly close as we shall see.

The continuity equation which relates the time change of the charge density to the divergence of the current density, provides the departure point for the proper derivation of the quantum current.

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0 \tag{2}$$

By integrating both sides of the continuity current over volume (d^3x) and using Gauss's theorem, one can show that the continuity equation is really just an elegant statement of charge conservation or the relationship between the rate of change of the charge within a surface and the sum of the currents flowing out of the surface.

$$\frac{\partial}{\partial t}\int\limits_{\mathcal{V}} d^3x\ \rho + \int\limits_{\mathcal{V}}\ d^3x\ \vec{\nabla}\cdot\vec{J} = 0$$

$$0 = \frac{\partial Q}{\partial t} + \int\limits_{\mathcal{S}} d\vec{a}\cdot\vec{J} = \frac{\partial Q}{\partial t} + I_{\mathrm{out}} \tag{3}$$

Rather than talking about the charge and current current density; one often removes a factor of e and talks about the probability density (PDF $= \rho$) and probability current. We know that the probability density is given by just $\rho = \Psi^*\Psi$ and can get a formula like the continuity equation by some simple, but clever manipulations of the time dependent Schrödinger Equation. We begin pre-multiplying the SE by Ψ^*:

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

We next pre-multiply the complex conjugate of the SE by Ψ and assume a real potential.

$$-i\hbar\Psi\frac{\partial\Psi^*}{\partial t} = -\frac{\hbar^2}{2m}\Psi\frac{\partial^2}{\partial x^2}\Psi^* + V(x)\Psi^*\Psi \tag{5}$$

Subtracting Eq. (5) from (4) we have:

$$i\hbar\left(\Psi^*\frac{\partial\Psi}{\partial t} + \Psi\frac{\partial\Psi^*}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\Psi^*\frac{\partial^2}{\partial x^2}\Psi - \Psi\frac{\partial^2}{\partial x^2}\Psi^*\right) \tag{6}$$

By applying the rules for differentiating a product it is easy to show:

$$\frac{\partial\Psi^*\Psi}{\partial t} = \left(\Psi^*\frac{\partial\Psi}{\partial t} + \Psi\frac{\partial\Psi^*}{\partial t}\right)$$

$$\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial}{\partial x}\Psi - \Psi\frac{\partial}{\partial x}\Psi^*\right) = \left(\Psi^*\frac{\partial^2}{\partial x^2}\Psi - \Psi\frac{\partial^2}{\partial x^2}\Psi^*\right) \tag{7}$$

Inserting the Eq. (7) expressions into Eq. (6) and dividing by $i\hbar$ we have:

$$\frac{\partial\Psi^*\Psi}{\partial t} + \frac{\partial}{\partial x}\frac{\hbar}{2mi}\left(\Psi^*\frac{\partial}{\partial x}\Psi - \Psi\frac{\partial}{\partial x}\Psi^*\right) = 0 \tag{8}$$

As you can see Eq. (8) is of the form of the 1 dimensional continuity Eq. (1) once one makes the identification:

$$\rho = \psi^*\psi \quad , \quad \vec{J} = \frac{\hbar}{2mi}\left(\Psi^*\frac{\partial}{\partial x}\Psi - \Psi\frac{\partial}{\partial x}\Psi^*\right) \rightarrow \frac{\hbar}{2mi}\left(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\right)$$

$$\vec{J} = \frac{\hbar}{m}\mathcal{I}m\left(\Psi^*\vec{\nabla}\Psi\right) \tag{9}$$

where the latter form follows from the observation that $a - a^* = 2i\,\mathcal{I}m(a)$ where $\mathcal{I}m()$ denotes an imaginary part.

In computing the current using Eq. (9) one must consider both the time dependence as well as the space dependence. In order to produce a non-vanishing current density, the wave function must have **a position dependent phase**. Otherwise, the phase of $\Psi(x,t)$ will be the same as the phase of $\vec{\nabla}\Psi(x,t)$ and therefore $\Psi^*\vec{\nabla}\Psi$ will be real. The current density for an electron in a stationary state of the form $\Psi(x,t) = \psi(x)\ \exp\left(-i\omega t\right)$ is zero since the phase dependence has no spatial dependence. This makes a great deal of sense since the PDF of a stationary state is time independent which indicates no charge movement or currents. A combination of two stationary states with different energies such as: $\Psi(x,t) = a\ \psi_1(x)\ \exp\left(-i\omega_1 t\right) + b\ \psi_2(x)\ \exp\left(-i\omega_2 t\right)$ will have a position dependent phase , an oscillating PDF, and a non-zero current density which you will explore in the exercises.

To reinforce the idea that a position dependent phase is required to support a quantum current, consider writing the wave function in polar form $\psi(x) = |\psi(x)|\ \exp(i\phi(x))$ where we have a real modulus function $|\psi(x)|$ and a real phase function $\phi(x)$. Using the chain rule it is easy to show that:

$$\vec{J} = \frac{\hbar}{m}|\psi(x)|^2\ \vec{\nabla}\phi(x) \tag{10}$$

Hence the quantum current is proportional to the gradiant of the phase – a constant phase implies no current.

A particularly simple example of a state with a current flow is a quantum traveling wave of the form: $\Psi(x,t) = a\ \exp\left(ikx - i\omega t\right)$. Direct substitution of this form into Eq. (9) or (10) gives us:

$$\vec{J} = (a^* a)\ \frac{\hbar k}{m}\ \hat{x} \tag{11}$$

A Strategy For Solving Tunneling Problems

We will limit ourselves to one-dimensional tunneling through a various potential barriers. An important consequence of working in one dimension is that the current must be the same at every point along the x-axis since there is no where for the charges to go. We can insure this automatically by using a single, stationary state wave function corresponding to a particle with a definite energy to describe the current flow everywhere. Let us see why this works. In one dimension, the (probability) continuity equation becomes:

$$\frac{\partial}{\partial t}\{\Psi^*\Psi\} + \frac{\partial J}{\partial x} = 0 \quad , \quad \frac{\partial}{\partial t}\{\Psi^*\Psi\} = 0 \ \text{ for a stationary state } \quad \rightarrow \frac{\partial J}{\partial x} = 0 \quad (12)$$

Eq. (12) implies that J is independent of position, and since it is constructed from a stationary state wave function, Eq. (9) tells us that J is independent of time. We thus automatically get a constant current with the same value *everywhere* along the x axis.

How do we find the stationary state wave function? Usually we choose a constant (often zero) potential region on the left of any barriers to "start" a wave function of the form $\psi = \exp(ikx) + r\ \exp(-ikx)$ where $k = \sqrt{2mE}/\hbar$. We think of the $\exp(ikx)$ piece as the incident wave which travels along the positive x axis and the $r\exp(-ikx)$ piece as the reflected wave. One can show† that the total current in this zero potential region (or any other region) is $J = \hbar k/m - |r|^2\hbar k/m$. We can think of the total current as the algebraic sum of the incident and reflected currents where each contribution is computed by Eq. (11). One then uses continuity of the wave function and derivative continuity to find the unknown r coefficient. The result of the calculation is generally expressed by a *reflection coefficient* $R \equiv |r|^2$ which is equivalent to $R = |J_r|/|J_i|$ where J_r is the reflected current due to $r\exp(-ikx)$ piece and J_i is the incident current due to the $\exp(ikx)$ piece. Our goal is to calculate R as a function of E which determines the k value we start with.

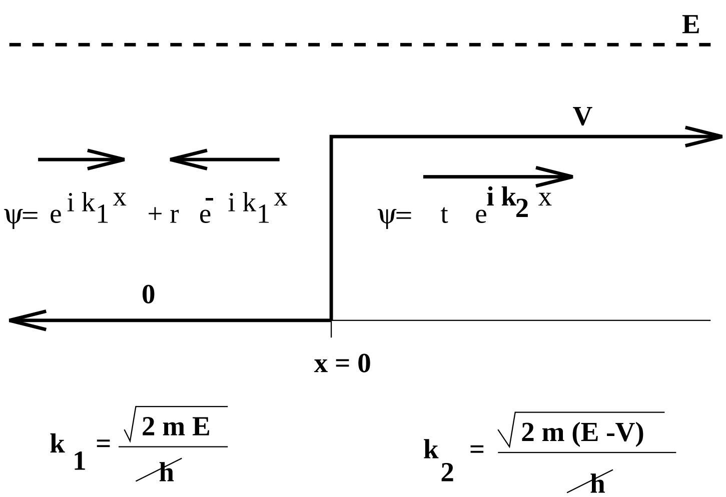
If it turns out that $R < 1$, there will be a net current at $x = +\infty$ (and everywhere else) which we will call the transmitted current or J_t. This will be a

† In homework you show that the interference between the incident and reflected parts of the wave function carries no current which is far from obvious without an explicit calculation

single current since we assume there is nothing at infinity to reflect this current. Current conservation reads $J_i + J_r = J_t$ or $|J_i| - |J_r| = |J_t|$ or dividing by $|J_i|$, $1 - R = T$ where T is the transmission coefficient defined as $T = |J_t|/|J_i|$. We will illustrate this approach in the next section.

The Quantum Curb

The quantum curb as illustrated below involves a traveling wave of the form $\exp{(ikx)}$ carrying an incident (probability) current $\vec{J} = \frac{k}{m}\,\hat{x}$ which travels to the right in the $x < 0$ region of zero potential. It strikes a potential step of height V at $x = 0$ producing both a reflected wave of amplitude r which travels to the left along with a transmitted wave of amplitude t which travels to the right. In order to insure traveling waves in both the $x > 0$ and $x < 0$ regions, the electron must be classically allowed and have sufficient energy such that $E > V$.



Following our strategy we write $\psi = \exp(ikx) + r\exp(-ikx)$ in our constant potential region at $x < 0$. We can then solve for r and t which are the amplitudes of the reflected and transmitted wave relative to the incident wave of unit amplitude by envoking continuity of ψ, Eq. (13), and its derivative, Eq. (14), at the point $x = 0$.

$$e^{ik_1 0} + r\ e^{-ik_1 0} = t\ e^{ik_2 0} \rightarrow 1 + r = t \tag{13}$$

$$\frac{\partial}{\partial x}\, e^{ik_1 x} + \frac{\partial}{\partial x}\, r\, e^{-ik_1 x} = \frac{\partial}{\partial x}\, t\, e^{ik_2 x}|_{x=0} \rightarrow \;\; ik_1 - ik_1\, r = ik_2\, t \rightarrow 1 - r = \frac{k_2}{k_1}\, t \quad (14)$$

Adding Eq. (13) and Eq. (14) we get

$$2 = 1 + \frac{k_2}{k_1}\, t \rightarrow t = \frac{2k_1}{k_1 + k_2} \quad (15)$$

$$\text{From} \;\; 1 + r = t \text{ we can find } r = 1 - \frac{2k_1}{k_1 + k_2} \rightarrow r = \frac{k_1 - k_2}{k_1 + k_2} \quad (16)$$

We note that $k_1 = \sqrt{2mE}/\hbar$ and $k_2 = \sqrt{2m(E - V)}/\hbar$ which means for the step up curb: $k_1 > k_2$ and $r > 0$. If the curb were a step down curve $r < 0$.

We turn next to the R and T coefficients. These are **not** the relative amplitudes t and r, but rather are the ratio of the currents carried by the transmitted or reflected waves over the incident wave. Following Eq. (11) we have:

$$T = \frac{(t^* t)\; k_2/m}{k_1/m} = \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad (17)$$

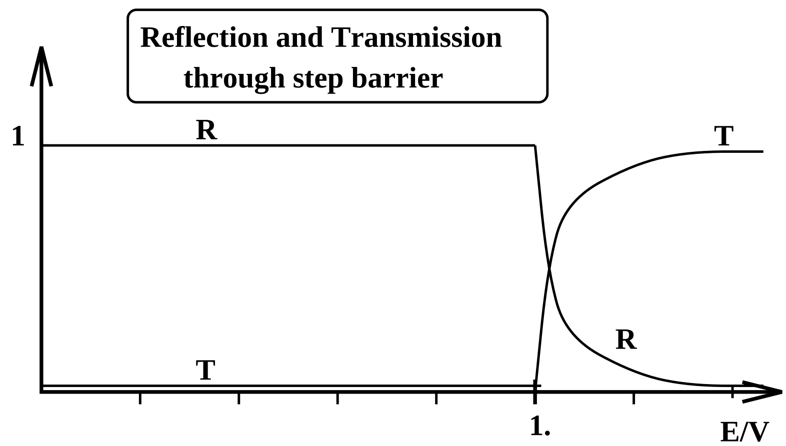
$$R = \frac{(r^* r)\; k_1/m}{k_1/m} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \quad (18)$$

Using algebra you can show from Eq. (17) and Eq. (18) that $T + R = 1$ as we expect. The current would not be conserved if we had (incorrectly) written the transmission coefficient as the just ratio of the transmitted over incident squared moduli ($T = t^* t$) rather than the correct expression $T = t^* t\; k_2/k_1$. The formula for the reflection and transmission coefficients for a light wave passing from air to glass is exactly the same as Eq.(17) and Eq. (18) which one gets from classical electrodynamics.

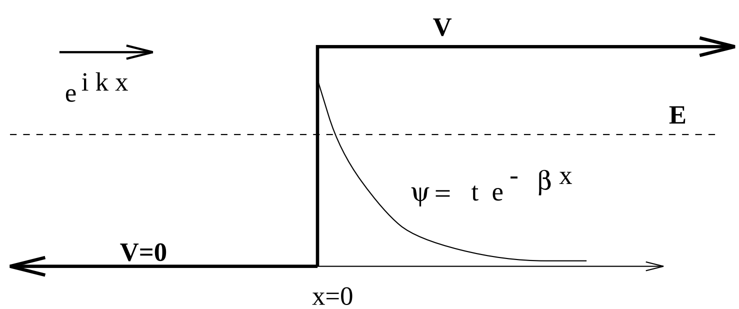
We can use $k_1 = \sqrt{2mE}/\hbar$ and $k_2 = \sqrt{2m(E-V)}/\hbar$ to write the transmission and reflection coefficients in terms of the dimensionless ratio E/V.

$$T = \frac{4\sqrt{E/V}\ \sqrt{E/V-1}}{\left(\sqrt{E/V}+\sqrt{E/V-1}\right)^2} \quad , \quad R = \frac{\left(\sqrt{E/V}-\sqrt{E/V-1}\right)^2}{\left(\sqrt{E/V}+\sqrt{E/V-1}\right)^2} \tag{19}$$

The below figure shows a sketch of the R and T coefficient as a function of E/V.



The above plot suggests that once $E < V$ there is 100 % reflection and 0 % transmission. This case is formally discussed in one of the exercises, but is reasonably easy to understand. If $E < V$, $x > 0$ becomes a classically forbidden region with an exponential wave function of the form $\psi = te^{-\beta x} = |t|\ e^{i\delta}\ e^{-\beta x}$.

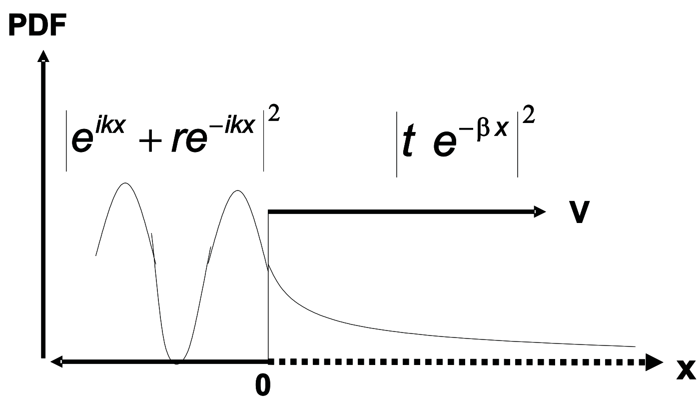


The current $\vec{J} = (\hbar/m)\mathcal{I}m\Big(\Psi^*\vec{\nabla}\Psi\Big)$ must vanish in this region since the complex phase is a constant (δ) independent of x. Informally there is no transmission current since the wave function of the electron exponentially dies away in the region $x > 0$ leaving no possibility of finding the electron at large values of x. Since there is no current at $x > 0$, there can be no current at $x < 0$ either which means the reflected current must cancel the incident current and thus $R = 1$.

It is interesting to compute the (unnormalized) PDF in the two regions. In the region $x > 0$ the PDF is of the form $\text{PDF}(x > 0) = |\psi(x)|^2 = |t|^2 \exp(-2\beta x)$. In the region $x < 0$ we have $\text{PDF(x} < 0) = \left|e^{ikx} + |r|\ e^{i\delta}\ e^{-ikx}\right|^2$ We have explicitly written the reflection amplitude as a modulus $|r|$ and a phase δ. In this case $|r| = 1$ and, as you show in homework, δ is a function of E/V. Using $|A + B|^2 = |A|^2 + |B|^2 + 2\text{Re}\{A^* B\} = |A|^2 + |B|^2 + 2\text{Re}\{B^* A\}$ we have:

$$\text{PDF(x} < 0) = 1 + |r|^2 + 2|r|\cos(2kx - \delta) = 2 + 2\cos(2kx - \delta) \qquad (20)$$

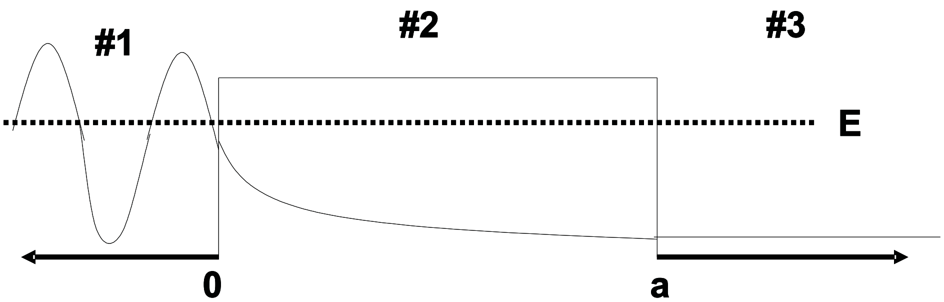
Below is a crude sketch of the PDF where the PDF has continuity and derivative continuity at $x = 0$. In the $x < 0$ region one has a standing wave pattern.



Quantum Tunneling

As we just saw, there is no transmission through a classically forbidden barrier step since beyond $x > 0$ we have a single, exponentially decaying wave function which cannot create the position dependent phase required to have a non-zero quantum current. If , on the other hand, we restore the potential back to ground as shown below, the classically forbidden region can have both $\exp(+\beta x)$ as well as $\exp(-\beta x)$ contributions. As long as the boundary condition equations give a different complex phase between these two contributions, the complex phase will develop a position dependence and the classically forbidden region will carry a current, implying there will be a current in the $x < 0$ region as well and hence $R < 1$, $T > 0$ and there will be a current at infinity.

Another way of looking at this is based on the fact that the current according to Eq. (9) is proportional to the wave function as well as its derivative. If there is just a classically forbidden region past $x > 0$, the wave function will die out to zero and there will be no possibility of a non-zero ψ at infinity. Since, $J \propto \psi^* \frac{\partial \psi}{\partial x}$ according to Eq. (9), this means there can be no quantum current at $x \to \infty$ and thus no net current anywhere. If , however, we restore the potential back to ground, we can "catch" the dying wave function before it totally decays away, and have thus have $\psi \neq 0$ at infinity and thus a current everywhere.



We have crudely sketched the PDF $= \psi^* \psi$ of the electron in the limit of low transmission. We can estimate the transmission coefficient in this limit by making use of the classically forbidden, quantum curb PDF's discussed in the last section. The PDF's in region #1 , #2, and #3 will be

$$\mathrm{PDF}_1 \approx 2+2\cos(2kx-\delta) \quad ; \quad \mathrm{PDF}_2 \approx |c|^2 e^{-2\beta x} \quad ; \quad \mathrm{PDF}_3 = |te^{ikx}|^2 = |t|^2 \quad (20b)$$

The region #1 PDF is approximate since we set $|r| = 1$ whereas $|r|$ is slightly less than 1 in the low transmission limit. The region #2 PDF is approximate since we threw away the $\exp(\beta x)$ piece that must be present in region #2 to convey the current but it should be small in this limit. We can now estimate $T = |t|^2$

by matching the approximate PDF's at $x = 0$ and $x = a$.

$$\mathrm{PDF}_1(0) = 2 + 2\cos(\delta) = f(E/V) = \mathrm{PDF}_2(0) = |c|^2 \rightarrow |c|^2 = f(E/V)$$

We write $\mathrm{PDF}_1(0) = f(E/V)$ since the phase δ is a function of E/V for the classically forbidden quantum current.

$$\mathrm{PDF}_2(a) = f(E/V)e^{-2\beta a} = \mathrm{PDF}_3(a) = |t|^2 \rightarrow T = f(E/V)e^{-2\beta a} \qquad (20c)$$

This is indeed the correct form of the exact solution when $\beta a \gg 1$ given by Eq. (26) that we discuss in the next section. We will show that $f(E/V)$ is a relatively smooth function that is approximately 1 meaning that the transmission coefficient is roughly $T \approx \exp -2\beta x$ where $\beta = \sqrt{2m(V-E)}/\hbar$. As we will argue later this means that the tranmitted current is very sensitive to very small (atomic scale) changes in a and the forbidden gap $V - E$. Here is an illustration. Consider an energy gap of $V - E = 2\ eV$. This is typical of the work function of metals which forms the barrier preventing metal electrons from escaping into space. The β corresponding to this work function is:

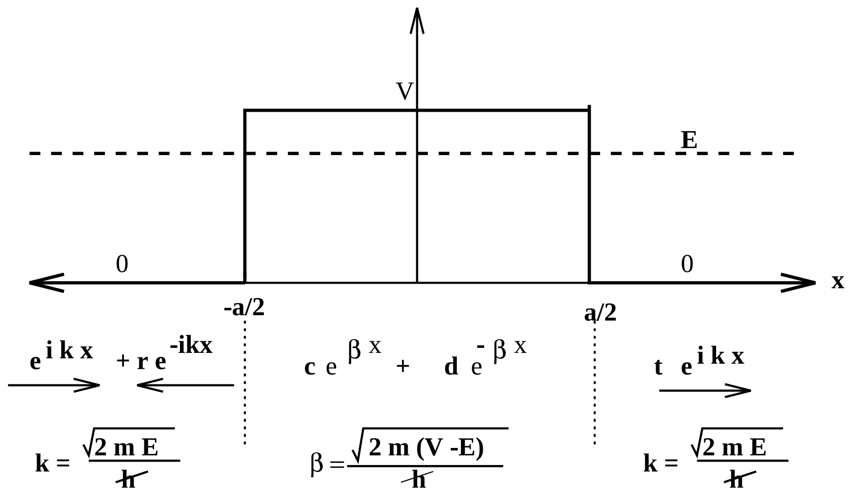
$$\beta = \frac{\sqrt{2m(V-E)}}{\hbar} = \frac{\sqrt{2mc^2(V-E)}}{\hbar c} = \frac{\sqrt{2(0.511 \times 10^6\ eV)(2\ eV)}}{197\ eVnm} = 7.26\, nm^{-1}$$

Now consider varying the tunneling length a from $a = 0.25\ nm$ to $a = 0.20\ nm$, the ratio of the tunneling current is:

$$\frac{T(0.20)}{T(0.25)} = \frac{f(E/V)\ \exp(-2(7.26)(0.20))}{f(E/V)\ \exp(-2(7.26)(0.25))} = e^{14.5\ (0.25-0.20)} = 2.1$$

To put this into perspective, we found that changing the tunneling length by the radius of a hydrogen atom (0.05 nm) changes the tranmission coefficient or tunneling current by 210 %. This extreme sensitivity of tunneling to distance changes on the scale of atomic dimensions forms the foundation of the STM or scanning tunneling microscope that we will describe later.

Formal Solution of the Classically Forbidden Barrier



In close analogy with our treatment of the step, in the region $x < -a/2$ we have an incident and reflected wave $\psi = e^{ikx} + r\ e^{-ikx}$. In the forbidden region, the wave function is constructed out of a decaying and growing exponential with unknown coefficients. We can envoke continuity and derivative continuity at the boundary $x = -a/2$ to obtain:

$$e^{-ika/2} + r\ e^{ika/2} = c\ e^{-\beta a/2} + d\ e^{+\beta a/2} \tag{21}$$

$$ik\ e^{-ika/2} - ik\ r\ e^{ika/2} = \beta\ c\ e^{-\beta a/2} - \beta d\ e^{+\beta a/2} \tag{22}$$

In the region $x > a/2$ we have a single transmitted wave and can envoke continuity and derivative continuity at the boundary $x = +a/2$ to obtain:

$$c\ e^{\beta a/2} + d\ e^{-\beta a/2} = t\ e^{ika/2} \tag{23}$$

$$\beta\ c\ e^{+\beta a/2} - \beta\ d\ e^{-\beta a/2} = ik\ t\ e^{ika/2} \tag{24}$$

Eq. (21) - Eq. (24) represent four equations in four unknowns: $(r \quad c \quad d \quad t)$. The solution to this series is not terribly instructive so I will just quote the results for the transmission coefficient:

$$T = \left(1 + \frac{\sinh^2(\beta a)}{4(E/V)(1-E/V)}\right)^{-1} \quad \text{where} \quad \beta = \frac{\sqrt{2m(V-E)}}{\hbar} \tag{25}$$

The reflection coefficient follows from $R = 1 - T$. To get some insight into this we will go to various limits.

The $\beta a \gg 1$ limit

In this limit $\sinh\beta \to \frac{1}{2}e^{\beta a} \gg 1$. This means that $\sinh^2(\;\;)/[\;\;]$ dominates the expression $1 + \sinh^2(\;\;)/[\;\;]$ and Eq. (25) becomes:

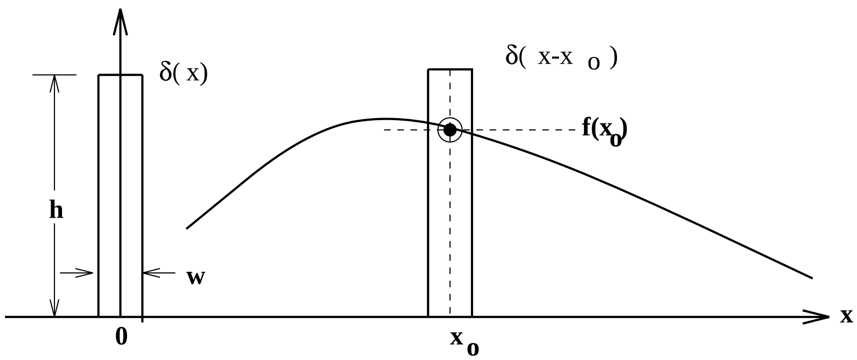
$$T \approx 16(E/V)(1-E/V) \;\; e^{-2\beta a} \tag{26}$$

This expression agrees with the form we deduced in Eq. (20c) in the $T \ll 1$ limit.

The Delta function limit

First a few words about δ-functions in case you haven't encountered them before. A δ function is a function with an infinitesimal width and an infinite height but a unit area. A force described as δ-function in time such as $F(t) = \delta(t)$ is known as a unit impulse which occurs at time $t = 0$. As you probably know from both mechanics and circuit theory; it is often relatively easy to describe a the behavior of a circuit or mechanical system to a voltage or force impulse. The same is true of quantum mechanical systems.

In quantum mechanics we often think of the a δ-function potential. We can think of this potential as a rectangular function of width w and height h in the limit that $w \to 0$, $h \to \infty$, and $wh = 1$ although there are many other limiting forms which approach the δ-function as well. The δ-function centered at $x = 0$ is written as $\delta(x)$. To shift the δ-function to the right so that it centers on x_o we translate the function by subtracting x_o from its argument or $\delta(x - x_o)$.



The operational definition of the δ-function is as follows:

$$\int_{x \in x_o} dx \ f(x) \ \delta(x - x_o) = f(x_o) \tag{28}$$

In words, the integral of the product of $f(x) \times \delta(x - x_o)$ over any interval containing the point x_o is just the function evaluated at x_o. Its easy to see how our rectangular representation of $\delta(x - x_o)$ has this property.

$$\int_{x \in x_o} dx \ f(x) \ \delta(x - x_o) = \lim_{w \to 0} \int_{x_o - w/2}^{x_o + w/2} dx \ h \times f(x) = wh \times f(x_o) = f(x_o) \tag{29}$$

δ-function potentials in the Schrödinger Equation

We write the time independent Schrödinger Equation for the case of a δ-function potential of strength g or $V(x) = g \ \delta(x - x_o)$. In writing this, we note that dimensions of strength g are energy $\times$ distance (*eg* $eV \cdot nm$) since the dimensions of $\delta(x - x_o)$ are distance^{-1} in order that $\int \ dx \ \delta(x - x_o) = 1$ (dimensionless).

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + g \ \delta(x - x_o)\psi = E\psi \tag{30}$$

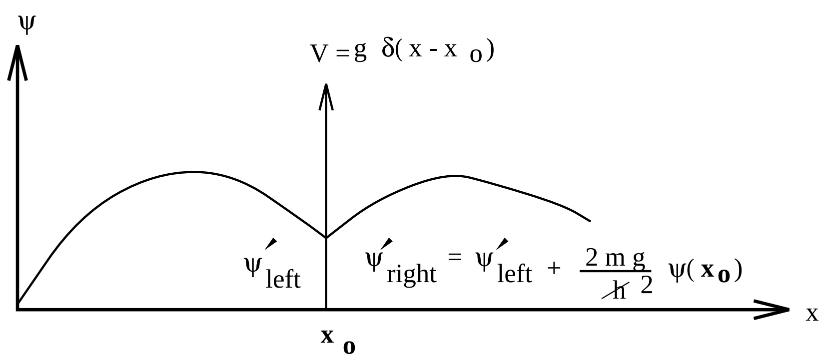
If we restrict ourselves to the region in an infinitesimal neighborhood of x_o, it is clear that $g\delta(x - x_o) \to \infty \gg E$ so we can ignore the righthand side.

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = g\ \delta(x - x_o)\psi \tag{31}$$

Integrating both sides of the equation from $x_o - \Delta \to X_o + \Delta$ where $\Delta \to 0$ we have:

$$\frac{\hbar^2}{2m} \int_{x_o-\Delta}^{x_o+\Delta} dx\ \frac{\partial^2 \psi}{\partial x^2} = \int_{x_o-\Delta}^{x_o+\Delta} dx\ g\ \delta(x - x_o)\psi = g\psi(x_o)$$

$$\frac{\partial \psi}{\partial x}_{x_o+\Delta} - \frac{\partial \psi}{\partial x}_{x_o-\Delta} = \frac{2mg}{\hbar^2}\psi(x_o) \tag{32}$$



Hence the δ-function potential creates a discontinuity in the slope of the wave function which is proportional to the δ-function strength and the value of ψ at the δ-function location. I will ask you in the exercises to apply Eq. (32) to compute the transmission coefficient through a δ-function barrier. Here is a check for you.

The $a \to 0$ but $Va = g$ limit of Eq. (25)

Lets consider this limit for:

$$T = \left(1 + \frac{\sinh^2(\beta a)}{4(E/V)(1 - E/V)}\right)^{-1} \quad \text{where} \quad \beta = \frac{\sqrt{2m(V - E)}}{\hbar}$$

Since Va is finite, $a\sqrt{V}$ or $\beta a \to 0$ and therefore $\sinh^2(\beta a) \to \beta^2 a^2$. We also have $4(E/V)(1 - E/V) \to 4E/V$ since $V \to \infty$. Hence

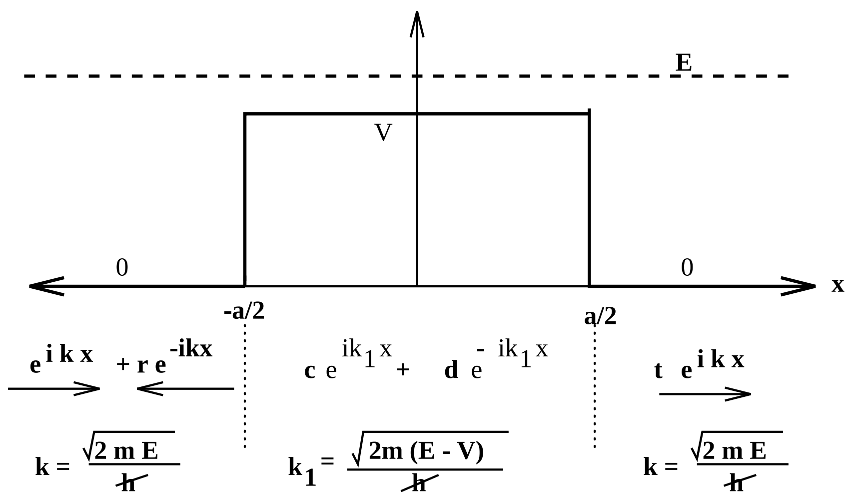
$$T = \left(1 + \frac{2ma^2(V-E)V}{4E\hbar^2}\right)^{-1} \to \left(1 + \frac{ma^2V^2}{2E\hbar^2}\right)^{-1} \tag{33}$$

Inserting $aV = g$ and $E = \hbar^2k^2/2m$ we have:

$$T = \left(1 + \frac{m^2g^2}{\hbar^4k^2}\right)^{-1} \tag{34}$$

Classically allowed barrier

We next consider the case of a traveling wave incident on a classically allowed barrier with $E > V$ as illustrated below.

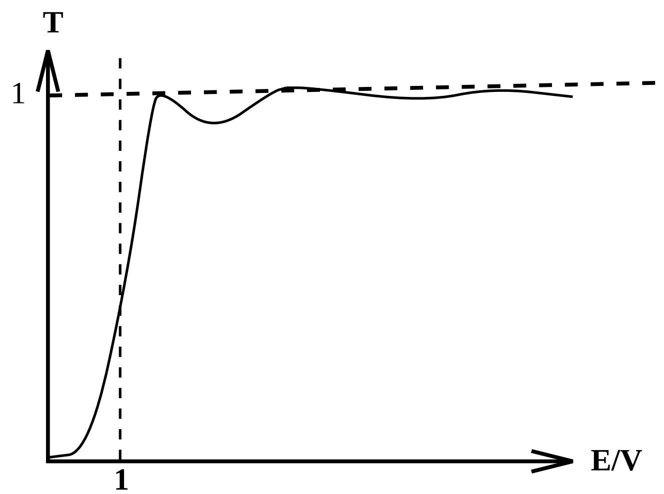


The transmission coefficient for this barrier is:

$$T = \left(1 + \frac{\sin^2(k_1a)}{4(E/V)(E/V-1)}\right)^{-1} \quad \text{where} \quad k_1 = \frac{\sqrt{2m(E-V)}}{\hbar} \tag{35}$$

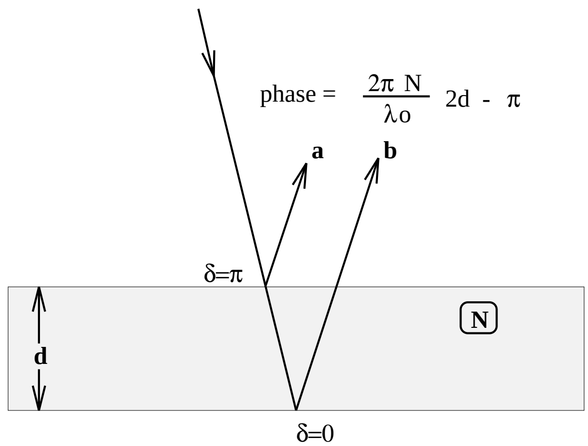
The real difference between this case and the classically forbidden case is the use of $c\ \exp(ik_1x) + d\ \exp(-ik_1x)$ rather than $c\ \exp(\beta x) + d\ \exp(-\beta x)$ for the wave function in the $0 < x < a$ region. Essentially the exponential argument $\beta \to ik_1$. We note that we can get to Eq. (35) from the forbidden T in Eq. (31) by the substitution $\sinh i\beta \to i \sin k_1$ which describes how a hyperbolic sine of an imaginary number is related to the usual sine.

We note from the form of Eq. (35), that we have perfect tranmission whenever $k_1 a = n\pi$, $n = 1, 2, ...$ This condition is equivalent to $n(\lambda_1/2) = a$ where λ_1 is the electron wavelength in the barrier region. Here is a crude sketch of the transmission coefficient as a function of E/V:



The phenemona of 100 % tranmission through a barrier at specific magic energies or wavelengths is often called **transmission resonance**. Examples occur in both atomic and nuclear physics. In atomic physics , one has the Ramsauer effect (discovered 1908) where noble gas atoms become nearly transparent to several volt electrons of of specific energies. A very similar phenomena, known as “size resonance”. occurs for several MeV neutrons which can pass transparently through the nucleus at resonant energies.

Transmission resonance at magic wavelengths also occurs in reflections of electromagnetic waves from thin films as shown below. We have angled the incident ray a bit for clarity but we will discuss the case of normal incidence.



The dielectric reflection from the top surface (**Ray a**) acquires a boundary phase shift of π, while the reflection from the bottom surface (**Ray b**) has no boundary phase shift but acquires an "distance" phase shift of $k_1(2d) = 2\pi d/\lambda$, where $\lambda = \lambda_o/N$ If $n(\lambda/2) = d$, the two reflected rays will cancel and destructively interfere leading to 100% transmission. This is essentially what happens in the quantum mechanical case as well: the waves reflected as the barrier is entered and exited interfere destructively.

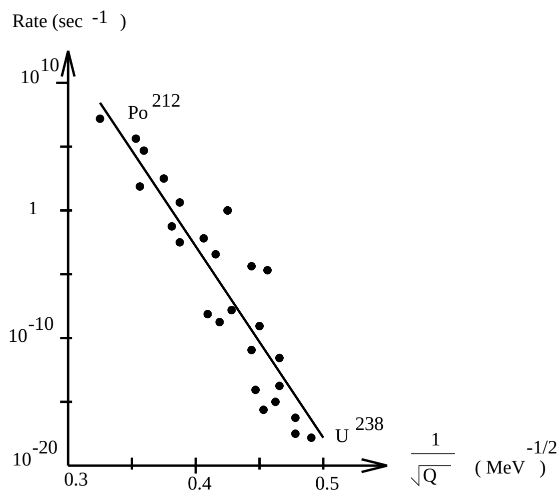
Quantum Tunneling in the Real World

There are a wide variety of real world phenemena which can be pictured in terms of tunneling processes.

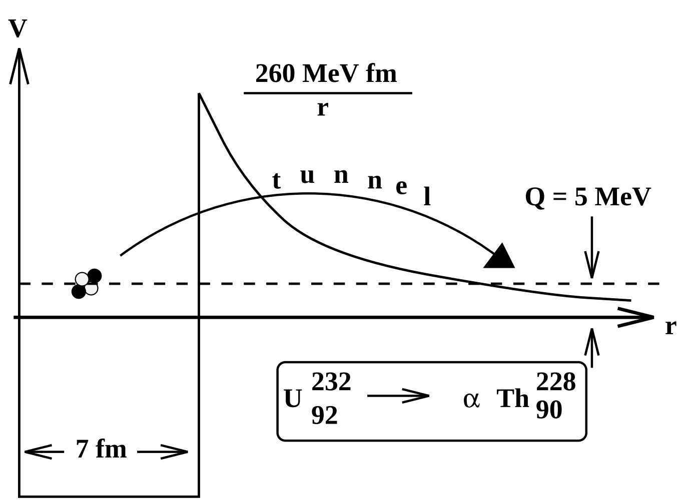
A example on the nuclear level involves alpha decay whereby a heavy parent nucleus becomes more stable by losing some electrical charge by ejecting an α particle. An example is provided by the decay of uranium isotopes:

$$U_{92}^{A} \rightarrow \alpha_2^4 + Th_{90}^{A-4}$$

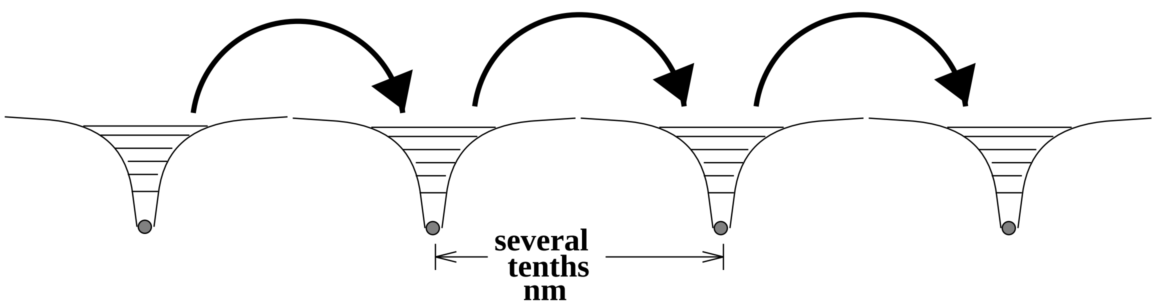
In this notation, A is the atomic weight (the number of neutrons and protons), the subscript is the atomic number (the number of protons). An α particle is a helium nucleus which is an unusually stable nucleus consisting of 2 neutrons and 2 protons. The half-life of the various radioactive isotopes depends exponentially on the energy release as crudely sketched below:



George Gamow in the 1930's proposed a quantum tunneling explanation for nuclear α decay. In this model, the α particle is initially bound by the strong interaction within a nuclear well created by the Thorium nucleus to form Uranium. The Uranium decays by having the α particle tunnel through the Coulomb barrier of the Thorium nucleus. As depicted below, the gap by which the tunneling is classically forbidden decreases as the energy release (Q) increases. The decay rate is proportional to the transmission coefficient through the barrier which depends exponentially on the energy gap.



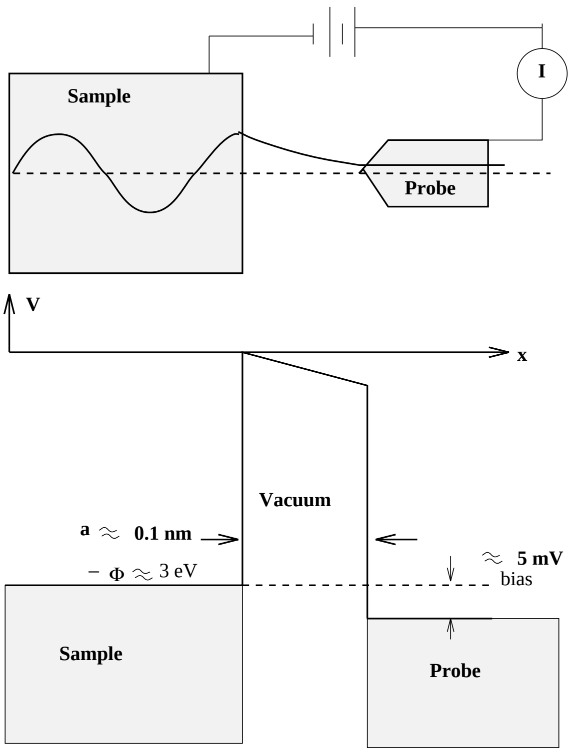
Nuclear α decay is controlled by very, small tranmission coefficients. At the other extreme, we consider the nearly free motion of conduction electrons through a metal. Although electrons are bound within individual metal atoms on quantum levels of the atomic discrete spectrum, they exhibit nearly free motion in a metal crystal where there is regularly spaced lattice of ions on a spacing of a few tenths of a nanometer.

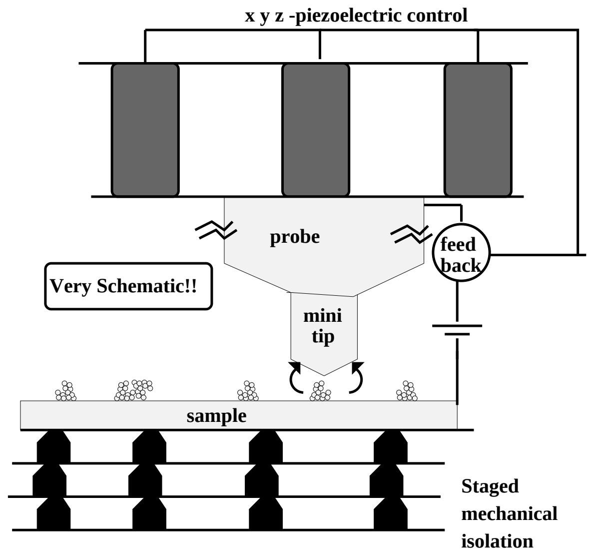


We can think of the loosely bound valence electrons in outer orbitals as jumping from ion to ion by quantum tunneling through fairly weak barriers owing to the narrow width and small depth of the effective interatomic barrier. We will discuss this in depth on our chapter on Crystals.

The Scanning Tunneling Microscope

A very impressive device which exploits the extreme sensitivity of quantum tunneling is called the Scanning Tunneling Microscope (STM) developed by Gerd Binnig and Heinrich Rohrer of the IBM Zurich Research Laboratory in 1981. They won the 1986 Nobel Prize for Physics for this achievement. The basic idea of the STM is sketched below:





The STM determines the distance between a surface and probe to atomic distance scales by measuring the quantum tunneling current of electrons leaving the sample and entering the probe. The quantum barrier to electron flow is essentially the work function of the metal. Recall from the photoelectric effect that it requires a certain minimum energy to photoeject an electron from a metal surface. In terms of a potential, we can say that the metal surface has a potential which lies below the potential of free space (vacuum). This minimum potential or work function (Φ) is typically several electron volts for most surfaces. Because of the work function, electrons will be bound within the surface. A naked surface will contain its electrons in analogy with a step barrier. The wavefunction outside the metal will be a classically forbidden wave function $\psi(x) = \exp(-\beta x)$ where $\beta = \sqrt{2m\Phi}/\hbar$, and there will be no electron current out of the surface. If one brings up a metal probe within a few atomic dimensions of the surface, one will form a quantum barrier rather than a step and it will be possible for electrons to quantum tunnel from the sample to the probe. Essentially the vacuum gap region (V = 0) acts as the quantum barrier to the electrons which lie at a few volts below vacuum potential.

The STM measures the gap between the surface and probe by measuring the size of the quantum tunneling current. In order to achieve a net current, it is necessary to induce an asymmmetry such that the tunneling current from the sample surface to the probe is not cancelled by an opposite tunneling current from the probe to the surface. To insure this asymmetry, the probe is typically biased a few millivolts below the surface being studied. The tunneling current is proportional to the surface electron density, the small bias potential, and the barrier transmission coefficient. This transmission coefficient depends exponentially on the gap between the surface and the probe. The probe is "scanned" across the sample surface in much the same way as a television raster pattern, and the tunnel current forms either a gray scale or pseudo-color picture of the surface height. It is possible to resolve variations in the tunneling current due to individual atoms changing the surface to probe barrier gap!

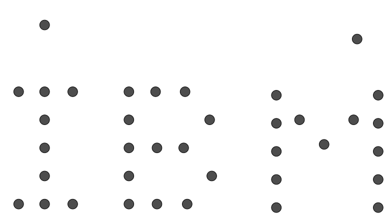
This is the concept but like any technological innovation, the devil is in the details. For example, in order to resolve individual atoms, one needs a probe tip which is only a few atoms wide. It is relatively easy to electochemically etch metals to achieve micron diameter wires, but this is about 10000 times too coarse. My understanding is that Binnig and Rohrer began with micron diameter tungsten needles which were then micro-pitted by placing them in a strong electric field which dislodge atoms on the surface leaving sharp points behind. The object was not to get one precisely polished micro-tip as depicted above, but one particularly sharp point which dominates the tunneling.

Another problem is mechanical oscillation due to room vibration. Typical vibration amplitudes are about a micron which is again 10000 times larger than the $\approx$0.1 nm required gap for good tunneling. These vibrations are damped by using a series of mechanical stages with carefully controlled natural vibration frequencies selected to block transmission of vibrations over a wide band width.

In addition they used copper plates and magnets designed to damp vibrations by dissipating eddy currents.

Finally one has the apparently formidable problem of controlling the probe position on the scale of atomic dimensions. The elegant solution employed by Binnig and Rohrer was to position the probe using a three point support consisting of three piezoelectric ceramics which expands or contracts by a few tenths of nanometer per applied volt. The tripod support allows the probe to be advanced to the surface (equal expansion of the ceramics) angled (unequal expansion) to affect a transverse scan. In one incarnation, one feeds the tunneling current through a control loop designed to maintain a constant tunnel current by having the probe follow the surface topography and thus maintain a constant gap. The display is then tied to the piezoelectric control current.

Not only can surfaces be measured, but the electrostatics of the probe can create forces which enable manipulation on the atomic level. A very impressive demonstration of this involved using an STM probe to nudge individual Xenon atoms to spell a word on a substate. Here is an crude artist's conception.



Because the distance between the probe and the sample is so small, there is little chance of air molecules slipping in between the tunneling gap. STM studies can be performed in air, oils, and even electrolytic solutions. This extends the reach of the instrument to physics, chemistry, engineering and microbiology.

Important Points

1. The quantum mechanical (probability) current density is given by

$$\vec{J} = \frac{\hbar}{2mi}\left(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\right) = \frac{\hbar}{m}\mathcal{I}m\left(\Psi^*\vec{\nabla}\Psi\right)$$

   The usual electric current density is equal to the charge $\times$ probability current density. In one dimension $\vec{\nabla} = \hat{x}\partial/\partial x$.

2. The traveling wave $\Psi(x,t) = a\ \exp(ikx - i\omega t)$ carries the probability current $\vec{J} = (a^*a)\ \frac{k}{m}\ \hat{x}$.

3. In barrier transmission problems we send in an incident traveling wave of the form $\psi(x) = e^{+ik_1x}$ which strikes the barrier producing a reflected wave (re^{-ik_1x}) and a transmitted wave $(\ te^{+ik_2x})$. The reflection and transmission coefficients are the ratios of the modulus of the reflected or transmitted currents to the incident current.

$$R = r^*r \quad , \quad T = \frac{k_2}{k_1}t^*t \quad , \quad R + T = 1$$

By matching boundary conditions for the case of a step boundary we obtained for a classically allowed step:

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

where k_1 and k_2 are the wave vectors in the two regions. For a classically forbidden step T=0 and R=1 but the reflected wave is phase shifted.

4. For a classically forbidden square bump barrier with a low transmission coefficient:

$$T \approx 16(E/V)(1 - E/V)\ \ e^{-2\beta a}$$

   where a is the width of the barrier and $\beta = \sqrt{2m(V-E)}/\hbar$.

5. One can have 100 % transmission through a classically allowed square bump barrier when the width is an integral number of half wavelengths (wavelengths in the barrier). This is the same condition for 100 % transmission through a thin film.

6. We discussed several real work applications of quantum tunneling. The conduction of electrons in a metal can be thought of as quantum tunneling between the closely spaced atoms of the lattice. In the low tranmission limit one has the Gamow model for α emission, and the scanning tunneling microscope. All these phenomena are hypersensitive to small differences in the energy or width of the barrier.