5 Quantum tunneling and simple harmonic motion

In this section we will apply the Schrödinger equation to understand the phenomenon of quantum tunneling. We will investigate quantum tunneling in action, i.e. via alpha particle decay of radioactive elements and via Scanning Tunneling Microscopy (STM). Finally, we will discuss the quantum description of simple harmonic motion and its application to molecular physics.

5.1 The potential barrier

We consider the case of a particle of energy E directed towards a potential barrier of height V_0 and width L (Figure 1).

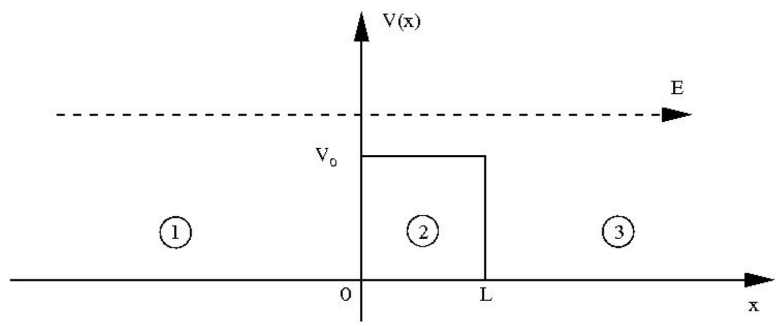

Figure 1: A schematic representation of a potential barrier.

We describe the potential $V(x)$ via

$$V(x) = \begin{array}{ll} 0 & x \leq 0 \\ V_0 & 0 < x < L \\ 0 & x \geq L \end{array} \tag{1}$$

5.1.1 Particle energy $E > V_0$

Classically the particle crosses the barrier every time. The velocity of the particle decreases when crossing the barrier. We see this as the total energy of the system can be written as

$$K = \frac{1}{2}mv^2 = E - V_0. \tag{2}$$

Our quantum mechanical model describes the particle as a wave function. We consider an analogy with optics: when light in the form of an electromagnetic wave travels from one medium to another, for instance from air to glass, the wavelength changes because of the changing index of refraction. Some of the incident light is transmitted and some is reflected. We extend this analogy to the quantum scale and describe the wave function in terms of an incident wave, a reflected wave and a transmitted wave. We can solve the Schrödinger equation for each wave function using the appropriate boundary conditions.

Once again we emphasize that classical physics predicts total transmission for $E > V_0$ and total reflection for $E < V_0$. As we will see, quantum mechanics predicts almost total transmission for $E \gg V_0$ and almost total reflection for $E \ll V_0$. It is in the regime $E \sim V_0$ that we expect unusual, or quantum, phenomena.

We can summarize the particle properties in each region of Figure 1:

$$\text{Region 1:}\quad p_1 = \sqrt{2mE} \;\Rightarrow\; k_1 = \frac{\sqrt{2mE}}{\hbar} \tag{3}$$

$$\text{Region 2:}\quad p_2 = \sqrt{2m(E-V_0)} \;\Rightarrow\; k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar} \tag{4}$$

$$\text{Region 3:}\quad p_3 = \sqrt{2mE} \;\Rightarrow\; k_3 = k_1 = \frac{\sqrt{2mE}}{\hbar} \tag{5}$$

We can also write down the time independent Schrödinger equation for each region:

$$\text{Region 1:}\quad \frac{\mathrm{d}^2\psi_1}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}E\,\psi_1 = 0 \quad\Rightarrow\quad \psi_1'' + k_1^2\psi_1 = 0 \tag{6}$$

$$\text{Region 2:}\quad \frac{\mathrm{d}^2\psi_2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E-V_0)\,\psi_2 = 0 \quad\Rightarrow\quad \psi_2'' + k_2^2\psi_2 = 0 \tag{7}$$

$$\text{Region 3:}\quad \frac{\mathrm{d}^2\psi_3}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}E\,\psi_3 = 0 \quad\Rightarrow\quad \psi_3'' + k_3^2\psi_3 = 0 \tag{8}$$

The wave functions then display solutions of the form

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \tag{9}$$

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x} \tag{10}$$

$$\psi_3 = Fe^{ik_1x} + Ge^{-ik_1x}, \tag{11}$$

Where we have intentionally dropped the use of the k_3 term. Each solution represents the time independent component of a travelling wave. If we consider the region 1 wave function, i.e. $\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$, and include the time dependence via $\Psi_1 = \psi_1 e^{-i\omega t}$ we obtain

$$\Psi_1 = Ae^{i(k_1x-\omega t)} + Be^{-i(k_1x+\omega t)}. \tag{12}$$

Amplitude	Direction
Ae^{ik_1x}	incident wave moving right
Be^{-ik_1x}	reflected wave moving left
Ce^{ik_2x}	barrier wave moving right
De^{-ik_2x}	barrier wave moving left
Fe^{ik_1x}	transmitted wave moving right
$Ge^{-ik_1x} = 0$	incident wave moving left

Table 1: Wave functions in the potential barrier problem.

Each term is referred to as an **amplitude**. The first amplitude (A) is a wave travelling towards $x > 0$, i.e. towards the right. We summarise each of the amplitudes in Table 1. Note that we impose the initial condition that the incident wave arrives from the left moving in the positive x-direction. The following boundary conditions must be satisfied

$$\psi_1(x=0) = \psi_2(x=0) \quad \text{and} \quad \psi_1'(x=0) = \psi_2'(x=0)$$

$$\psi_2(x=L) = \psi_3(x=L) \quad \text{and} \quad \psi_2'(x=L) = \psi_3'(x=L)$$

The boundary conditions generate four equations

$$A + B = C + D \tag{13}$$

$$ik_1A - ik_1B = ik_2C - ik_2D \tag{14}$$

$$Ce^{ik_2L} + De^{-ik_2L} = Fe^{ik_1L} \tag{15}$$

$$ik_2Ce^{ik_2L} - ik_2De^{-ik_2L} = ik_1Fe^{ik_1L} \tag{16}$$

We are now in a position to define the **transmission** and **reflection probabilities**:

1. Transmission probability

$$T \equiv \frac{\psi^*_{trans}\psi_{trans}}{\psi^*_{incid}\psi_{incid}} = \frac{F^*e^{-ik_1x}Fe^{ik_1x}}{A^*e^{-ik_1x}Ae^{ik_1x}} = \frac{F^*F}{A^*A}. \tag{17}$$

2. Reflection probability

$$R \equiv \frac{\psi^*_{ref}\psi_{ref}}{\psi^*_{incid}\psi_{incid}} = \frac{B^*e^{ik_1x}Be^{-ik_1x}}{A^*e^{-ik_1x}Ae^{ik_1x}} = \frac{B^*B}{A^*A}. \tag{18}$$

We can further specify that $R + T = 1$. The calculation of T requires the boundary conditions to obtain an expression for F/A.

1. Eliminate B by taking $ik_1\times$ Eqn. 13 + Eqn. 14:

$$2ik_1 A = i(k_1 + k_2)C + i(k_1 - k_2)D. \tag{19}$$

2. Eliminate D by taking $ik_2\times$ Eqn. 15 + Eqn. 16:

$$2ik_2 C e^{ik_2 L} = i(k_1 + k_2)F e^{ik_1 L}. \tag{20}$$

3. Eliminate C by taking $ik_2\times$ Eqn. 15 − Eqn. 16:

$$2ik_2 D e^{-ik_2 L} = -i(k_1 - k_2)F e^{ik_1 L}. \tag{21}$$

4. Substitute Equations 20 and 21 into Equation 19 to obtain

$$2ik_1 A = \frac{i^2(k_1+k_2)^2\, F e^{ik_1 L}}{2ik_2 e^{ik_2 L}} - \frac{i^2(k_1-k_2)^2\, F e^{ik_1 L}}{2ik_2 e^{-ik_2 L}} \tag{22}$$

$$\frac{A}{F} = \frac{e^{ik_1 L}}{4k_1 k_2}[(k_1+k_2)^2 e^{-ik_2 L} - (k_1-k_2)^2 e^{ik_2 L}] \tag{23}$$

$$= \frac{e^{ik_1 L}}{4k_1 k_2}[(k_1^2 + 2k_1 k_2 + k_2^2)e^{-ik_2 L} - (k_1^2 - 2k_1 k_2 + k_2^2)e^{ik_2 L}] \tag{24}$$

5. We next make use of the following trigonometric relations

$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \qquad \sin x = \frac{e^{ix} - e^{-ix}}{2i}, \tag{25}$$

in order to write

$$\frac{A}{F} = \frac{e^{ik_1 L}}{4k_1 k_2}(4k_1 k_2 \cos(k_2 L) - 2i(k_1^2 + k_2^2)\sin(k_2 L)). \tag{26}$$

6. We next inspect the expression for A/F and notice that

$$\frac{A}{F} \quad \text{looks like} \quad e^{i\theta}(a - ib),$$

$$\left(\frac{A}{F}\right)^* \quad \text{looks like} \quad e^{-i\theta}(a + ib),$$

$$\left(\frac{A}{F}\right)^* \left(\frac{A}{F}\right) \quad \text{looks like} \quad a^2 + b^2.$$

Therefore, we write

$$\left(\frac{A}{F}\right)^* \left(\frac{A}{F}\right) = \frac{1}{16k_1^2k_2^2}(16k_1^2k_2^2\cos^2(k_2L) + 4(k_1^2+k_2^2)^2\sin^2(k_2L)) \tag{27}$$

$$= \cos^2(k_2L) + \frac{(k_1^2+k_2^2)^2\sin^2(k_2L)}{4k_1^2k_2^2} \tag{28}$$

$$= 1 - \sin^2(k_2L) + \frac{(k_1^2+k_2^2)^2\sin^2(k_2L)}{4k_1^2k_2^2} \tag{29}$$

$$= 1 + \left(\frac{(k_1^2+k_2^2)^2 - 4k_1^2k_2^2}{4k_1^2k_2^2}\right)\sin^2(k_2L) \tag{30}$$

$$= 1 + \left(\frac{(k_1^2-k_2^2)^2}{4k_1^2k_2^2}\right)\sin^2(k_2L) \tag{31}$$

$$\frac{1}{T} = 1 + \left(\frac{\left(\frac{2mE}{\hbar^2} - \frac{2m(E-V_0)}{\hbar^2}\right)^2}{4\cdot\frac{2mE}{\hbar^2}\cdot\frac{2m(E-V_0)}{\hbar^2}}\right)\sin^2(k_2L) \tag{32}$$

$$\frac{1}{T} = 1 + \frac{\left(\frac{2mV_0}{\hbar^2}\right)^2}{16\frac{m^2}{\hbar^4}E(E-V_0)}\sin^2(k_2L) \tag{33}$$

$$T = \left(1 + \frac{V_0^2\sin^2(k_2L)}{4E(E-V_0)}\right)^{-1} \quad \text{for } E > V_0. \tag{34}$$

7. The transmission formula predicts two distinct outcomes for $E > V_0$:

   (a) We note that $T = 1$ for $k_2L = n\pi$ where $n = 1, 2, \ldots$, i.e. the result looks like the classical outcome where an exact number of wavelengths fit within the width of the potential barrier.

   (b) In all other cases we note that $T < 1$ and $R > 0$, i.e. there is a certain probability that the particle will be reflected even when it has sufficient energy to clear the barrier.

5.1.2 Particle energy $E < V_0$

Classically, a particle of energy $E < V_0$ is always reflected by the potential barrier. When we consider a particle described by a quantum wave function we observe a small but finite possibility for the particle to "tunnel" through the barrier and continue on the other side. The analysis of the

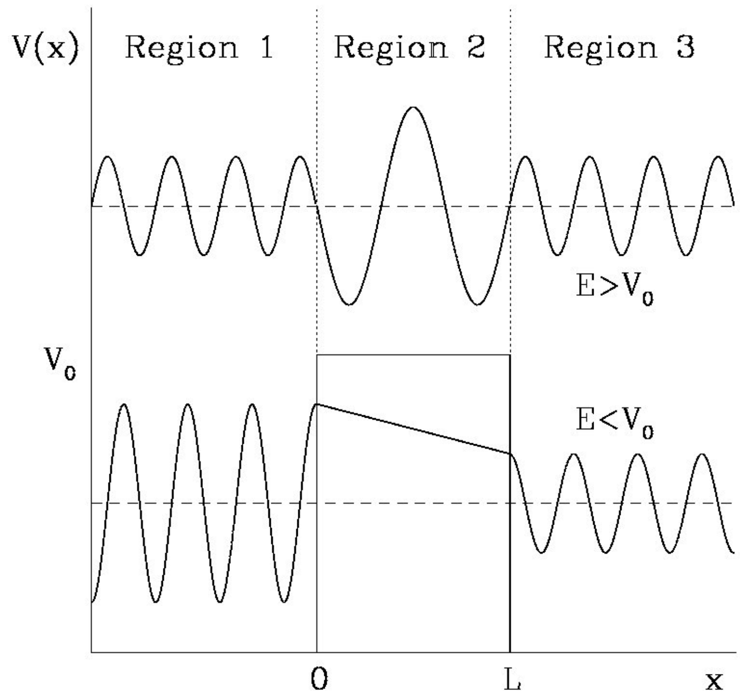

Figure 2: Wave function solutions across a potential barrier.

situation $E < V_0$ follows the previous analysis for $E > V_0$ with the exception that we must modify the wave number within the barrier (Equation 7)

$$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar} = \frac{\sqrt{-2m(V_0 - E)}}{\hbar}, \tag{35}$$

which is now an imaginary quantity. We therefore define $k_2 = i\kappa$ where

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}, \tag{36}$$

and the wave function within region 2 may be re-written as

$$\psi_2 = Ce^{-ik_2 x} + De^{ik_2 x} = Ce^{\kappa x} + De^{-\kappa x}, \tag{37}$$

i.e. the wave function within the barrier is now described by an exponential, rather than an oscillatory, term. When computing the transmission and reflection probabilities for $E < V_0$, the algebra follows that used previously until we reach Equation 26 and take the complex conjugate, i.e.

$$\frac{A}{F} = \frac{e^{ik_1L}}{4k_1k_2}\left(4k_1k_2\left[\frac{e^{ik_2L}+e^{-ik_2L}}{2}\right] - 2i(k_1^2+k_2^2)\left[\frac{e^{ik_2L}-e^{-ik_2L}}{2i}\right]\right). \tag{38}$$

At this point we let $k_2 = i\kappa$ and write

$$\frac{A}{F} = \frac{e^{ik_1L}}{4k_1\kappa}\left(4k_1\kappa\left[\frac{e^{-\kappa L}+e^{\kappa L}}{2}\right] - 2i(k_1^2-\kappa^2)\left[\frac{e^{-\kappa L}-e^{\kappa L}}{2i}\right]\right) \tag{39}$$

$$= \frac{e^{ik_1L}}{4k_1\kappa}(4k_1\kappa\cosh(\kappa L) + 2(k_1^2-\kappa^2)\sinh(\kappa L)), \tag{40}$$

where we have used the trigonometrical relations

$$\cosh x = \frac{e^x+e^{-x}}{2} \qquad \sinh x = \frac{e^x-e^{-x}}{2}. \tag{41}$$

We can now take the complex conjugate of the expression A/F and write

$$\left(\frac{A}{F}\right)^*\left(\frac{A}{F}\right) = \frac{1}{16k_1^2\kappa^2}(16k_1^2\kappa^2\cosh^2(\kappa L) + 4(k_1^2-\kappa^2)^2\sinh^2(\kappa L)). \tag{42}$$

Note that cross terms involving $\cosh(x)\sinh(x)$ equal zero. Furthermore, by using $\cosh^2(x) - \sinh^2(x) = 1$ we may write the inverse transmission probability as

$$\frac{1}{T} = 1 + \sinh^2(\kappa L) + \frac{(k_1^2-\kappa^2)^2}{4k_1^2\kappa^2}\sinh^2(\kappa L) \tag{43}$$

$$= 1 + \left(\frac{4k_1^2\kappa^2 + (k_1^2-\kappa^2)^2}{4k_1^2\kappa^2}\right)\sinh^2(\kappa L) \tag{44}$$

$$= 1 + \left(\frac{(k_1^2+\kappa^2)^2}{4k_1^2\kappa^2}\right)\sinh^2(\kappa L) \tag{45}$$

$$= 1 + \left(\frac{\left(\frac{2mE}{\hbar^2} + \frac{2mV_0}{\hbar^2} - \frac{2mE}{\hbar^2}\right)^2}{4\cdot\frac{2mE}{\hbar^2}\cdot\frac{2m(V_0-E)}{\hbar^2}}\right)\sinh^2(\kappa L) \tag{46}$$

$$= 1 + \frac{(2mV_0)^2}{16m^2E(V_0-E)}\sinh^2(\kappa L) \tag{47}$$

$$\text{i.e.}\quad T = \left(1 + \frac{V_0^2\sinh^2(\kappa L)}{4E(V_0-E)}\right)^{-1}. \tag{48}$$

The fact that T takes a non-zero value indicates the finite probability that the particle tunnels through the barrier and continues on the other side. What form does the tunneling probability take? Assuming $\kappa L \gg 1$ we may write

$$T = 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2\kappa L}, \tag{49}$$

i.e. the tunneling probability decays exponentially for a thicker potential barrier. As $\kappa \propto \sqrt{V_0 - E}$ we note that the tunneling probability is more sensitive to the thickness of the barrier L than its height V_0.

T-Rex Example 6.14: A beam of electrons is accelerated through a potential of 5 V toward a potential barrier of width 0.8 nm and height 10 eV. What fraction of the electrons tunnel through the barrier?

The exact expression for the tunneling probability is given in Equation 48. We begin by determining the value of κ

$$\begin{aligned}
\kappa &= \frac{\sqrt{2m(V_0 - E)}}{\hbar} \\
&= \frac{\sqrt{2mc^2(V_0 - E)}}{\hbar c} \\
&= \frac{\sqrt{2 \times (511 \times 10^3 \text{ eV}) \times (10 - 5 \text{ eV})}}{197.3 \text{ ev nm}} \\
&= 1.15 \times 10^{-10}\text{m}^{-1}
\end{aligned}$$

Therefore,

$$\kappa L = 1.15 \times 10^{-10} \times 8 \times 10^{-10} = 9.2.$$

Using the exact expression for the tunneling probability we obtain

$$\begin{aligned}
T &= \left[1 + \frac{(10 \text{ eV})^2 \sinh^2(9.2)}{4(5 \text{ eV})(5 \text{ eV})}\right]^{-1} \\
&= 4.1 \times 10^{-8}.
\end{aligned}$$

If we use the approximate form of the tunneling probability, assuming $\kappa L \gg 1$ we obtain

$$\begin{aligned}
T &= 16\left(\frac{5 \text{ eV}}{10 \text{ eV}}\right)\left(1 - \frac{5 \text{ eV}}{10 \text{ eV}}\right)e^{-18.4} \\
&= 4.1 \times 10^{-8}.
\end{aligned}$$

The two formulae give the same answer and we see that the approximation $\kappa L \gg 1$ is valid.

End of T-Rex Example 6.14

We can understand quantum tunneling in terms of the **uncertainty principle**. Within the barrier the particle wave function is dominated by the $e^{-\kappa x}$ term. The probability of the particle existing within the barrier is $|\psi_2^2| \approx e^{-2\kappa x}$. We can define a distance $\Delta x = \kappa^{-1}$ over which the probability density describing the particle within the barrier decreases markedly, i.e. $e^{-2\kappa x} = e^{-2} = 0.14$. If we insert this value for Δx into the uncertainty principle, we obtain $\Delta p \geq \hbar/\Delta x = \hbar\kappa$. The minimum kinetic energy required over this interval is

$$K_{min} = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2\kappa^2}{2m} = V_0 - E. \tag{50}$$

Therefore the uncertainty in the kinetic energy of the particle tunneling through the barrier is equal to the energy deficit required to cross the barrier. In a sense, the particle is able to penetrate a short distance into the barrier by "borrowing" energy from the uncertainty principle.

5.2 Alpha particle decay and quantum tunneling

Alpha particle decay occurs from heavy, radioactive nuclei. Although many types of nuclei emit alpha particles, the rate of emission varies from nucleus to nucleus by a factor of order 10^{13}. However, the energies of the emitted alpha particles are remarkably constant, being of order 4 to 8 MeV. These large variations in emission transparency can be understood in terms of the probability for the alpha particles to tunnel through the nuclear binding potential (Figure 3).
Within the nuclear radius r_N the combination of the strong nuclear force (attractive) and Coulomb force of the nuclear protons (repulsive) approximates to a zero net potential. However, to escape the nucleus the alpha particle must break through the Coulomb barrier formed by the nuclear protons. The height of the Coulomb barrier can be equal to several times the KE of the alpha particle ($\sim$ 5 MeV) – effectively trapping the alpha particle in the nucleus. However, the alpha particle has a small chance of tunneling through the nuclear Coulomb barrier and, as the transmission probability $T \propto e^{-2\kappa L}$, small changes in the barrier height and width can produce a change in the transmission probability of many orders of magnitude.

T-Rex Example 6.17: Consider alpha particle emission from a ^{238}U nucleus. The alpha particle has a KE of 4.2 MeV and is initially contained within a nuclear radius of $r_N = 7 \times 10^{-15}$m. Find the barrier height and the distance the alpha particle must tunnel through. Use a suitable approximation to compute the tunneling probability.

1. We compute the barrier height by determining the Coulomb potential at the nuclear radius, i.e.

$$V_c(r = r_N) = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r_N}$$

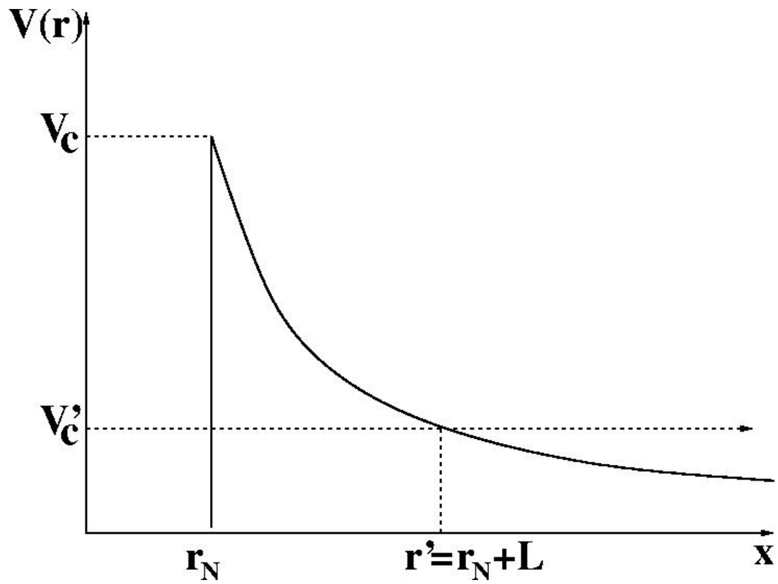

Figure 3: Alpha particle tunneling.

$$= \frac{(2)(90)(1.6\times10^{-19}\mathrm{C})^2(9\times10^9\ \mathrm{Nm^2C^{-2}})}{7\times10^{-15}\ \mathrm{m}} \times \frac{1}{1.6\times10^{-13}\ \mathrm{J\ MeV^{-1}}}$$

$$= 37\ \mathrm{MeV}.$$

2. The alpha particle will have effectively escaped the nucleus when it reaches a radius r' given by

$$KE = 4.2\ \mathrm{MeV} = \mathrm{V_c(r')} = \frac{\mathrm{Z_1Z_2e^2}}{4\pi\epsilon_0\mathrm{r'}}.$$

We can solve this in a fairly straightforward fashion by noting that

$$V_c \times r = \frac{Z_1Z_2e^2}{4\pi\epsilon_0} = \text{constant},$$

i.e.,

$$V_c(r_N)\,r_N = V_c(r')\,r',$$

and

$$r' = \frac{V_c(r_N)}{V_c(r')}r_N = \frac{V_c(r_N)}{KE}r_N$$

$$= \frac{37 \text{ MeV}}{4.2 \text{ MeV}} \times 7 \times 10^{-15} \text{ m}$$

$$= 6.2 \times 10^{-14} \text{ m} = 62 \text{ fm}.$$

The width of the barrier through which the alpha particle must tunnel is therefore

$$L = r' - r_N = 62 \text{ fm} - 7 \text{ fm} = 55 \text{ fm}.$$

3. Now modeling the barrier as a square well of height V_c and width L is pretty unrealistic – especially given the exponential dependence of the tunneling probability on κ and L (Figure 4). A reasonably accurate model would see the barrier split into five bins of width 11 fm. We can calculate the transmission probability of each bin and the total transmission probability will be given by their product.

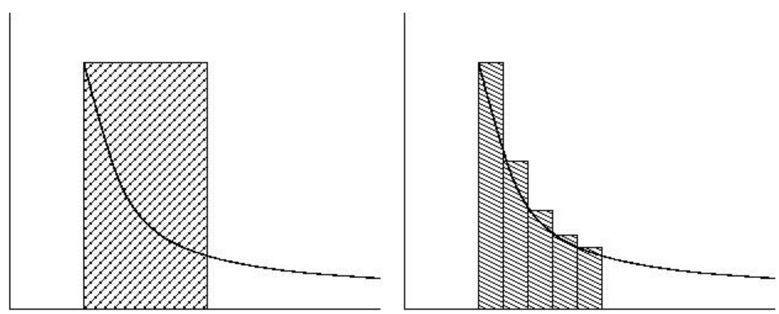

Figure 4: Modeling the potential barrier.

We compute the value of κ explicitly for the first bin and then tabulate the remaining results (Table 2).

$$\begin{aligned}
\kappa_1 &= \frac{\sqrt{2m(V_1 - E)}}{\hbar} \\
&= \frac{\sqrt{2mc^2(V_1 - E)}}{\hbar c} \\
&= \frac{\sqrt{(2)(3727 \text{ MeV})(\text{V}_1 - 4.2 \text{ MeV})}}{197.3 \text{ MeV fm}} \\
&= \frac{\sqrt{(2)(3727 \text{ MeV})(20.7 \text{ MeV} - 4.2 \text{ MeV})}}{197.3 \text{ MeV fm}} \\
&= 1.7 \text{ fm}^{-1}.
\end{aligned}$$

We then form the quantity κL, i.e.

$$\kappa_1 L = 1.7 \text{ fm}^{-1} \times 11 \text{ fm} = 18.7 \gg 1.$$

We can therefore compute the transmission probability as

$$\begin{aligned} T_1 &= 16\frac{E}{V_1}\left(1-\frac{E}{V_1}\right)e^{-2\kappa_1 L} \\ &= 16\frac{4.2}{20.7}\left(1-\frac{4.2}{20.7}\right)e^{-37.4} \\ &= 1.6\times 10^{-16}. \end{aligned}$$

r (fm)	V (MeV)	κ (fm^{-1})	κL	$\log T$
12.5	20.7	1.7	18.7	-15.8
23.5	11.0	1.1	12.5	-10.2
34.5	7.5	0.8	8.7	-7.0
45.5	5.7	0.5	5.9	-4.6
56.5	4.6	0.3	3.7	-3.1

Table 2: Transmission probabilities across the Coulomb barrier.

The total transmission probability is $T = 1.6 \times 10^{-41}$. Though this seems like a prohibitively small escape probability, we must consider how many "escape attempts" the alpha particle will make. A 4.2 MeV alpha particle is non-relativistic. Its velocity is therefore

$$v = \sqrt{\frac{2K}{m}} = \sqrt{\frac{2\times 4.2 \text{ MeV}}{3727 \text{ MeV}/c^2}} = 0.047\ c = 1.4\times 10^7 \text{ms}^{-1}.$$

The diameter of the uranium nucleus is $2\ r_N$ and the alpha particle will cross the nucleus in a time

$$t = \frac{2\ r_N}{v} \simeq 10^{-21} \text{ s}.$$

If this is the time required to make one escape attempt, and the alpha particle requires 10^{41} attempts in order to escape, it will escape on average after of order 10^{20} seconds. The observed half-life of ^{238}U is of order 10^{17} seconds (about 4.5 billion years) – our approximate approach is therefore not "too" bad.

5.3 Scanning Tunneling Microscopes (STM)

STM provides a method to image atomic structures on scales down to a few tenths of a nanometre. To understand the advances made by STM, it is worthwhile considering for a moment Scanning Electron Microscopes (SEM).

SEM has existed as a techniques for about 80 years. To image a source you must first coat it in a thin gold foil. The "light" source is an electron beam fired at the target. The electrons in the beam interact with the conduction electrons in the gold foil and scatter off into a detector that surrounds the target. By studying the varying scattering angle as you move the electron beam around the target you build up a "picture" of the target (in this case a termite). However, the resolution achievable with SEM is limited by the De Broglie wavelength of the electrons in the beam and its energy resolution, $\Delta E/E$, which translates to $\Delta\lambda/\lambda$. In contrast to this STM (Figure 5) uses electron tunneling to map out atomic structures on two dimensional surfaces – typically for conducting and semi-conducting materials.

• A STM consists of a very sharp (e.g. single atoms at the tip) conducting stylus which is moved over the target material a small distance above it, i.e. a distance L.

• Conducting electrons in the target material have some thermal energy E and would like to jump across the distance L to the tip. However, they are prevented from doing so by the work function of the material, ϕ, i.e. $E < \phi$.

• STM works by encouraging the conduction electrons in the target material to tunnel across this barrier. This is achieved by applying an accelerating potential V across the material-tip distance. The potential is adjusted such that $E < \phi - V$ but this time only by a very small amount. Applying the potential reduces κ and therefore maximises the transmission probability (and thus the tunneling current) for a given L.

• The potential is kept constant and the transmission probability is $T \propto e^{-2\kappa L}$. A constant potential ensures that κ is constant and small changes in L result in large changes in the transmission probability.

• As the received tunneling current $I \propto T$, one can now measure the varying height of the tip above the surface. In practice though the height of the tip is varied in order to keep the tunneling current constant but the height variation is measured nonetheless.

• This method is very sensitive to the tunneling gap. Although the tunneling current can be as small as 10^{-12}A, a change of only 0.4nm can cause the current to vary by a factor 10^4.

5.4 Simple Harmonic Motion

Simple Harmonic Oscillators (SHOs) occur commonly in nature. The familiar example is of a mass suspended on a string. However, on the quantum scale pairs of atoms in diatomic molecules or arrays of atoms bound into a lattice structure act as SHOs. SHM results from the basic form of the potential acting on a massive particle. For example, consider a mass m attached to a spring described by a spring constant κ that is free to move in the x-direction. The resulting force about

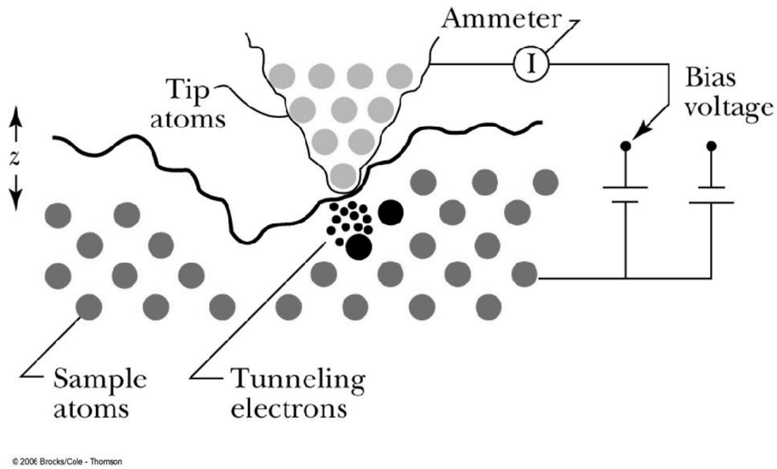

Figure 5: Scanning tunneling microscopy in action.

the equilibrium position x_0 is

$$F = -\kappa(x - x_0) \tag{51}$$

and the potential energy stored in the spring (effectively the potential acting on the particle) is

$$V = \frac{\kappa(x - x_0)^2}{2}. \tag{52}$$

Consider a simple quantum potential: an atom bound in a lattice that is at equilibrium at x_0 and experiences a potential $V(x)$ that depends upon the separation $(x - x_0)$ (Figure 6). For small displacements about the equilibrium position we can expand the potential as a Taylor series, i.e.

$$V(x) = V_0 + V_1(x - x_0) + \frac{1}{2}V_2(x - x_0)^2 + \ldots \tag{53}$$

If $x = x_0$ is an equilibrium position then there must exist a minimum in the potential

$$\frac{\mathrm{d}V}{\mathrm{d}x} = 0 \ \text{ at } \ x = x_0. \tag{54}$$

This requires that $V_1 = 0$ and by re-scaling the zero point of the potential energy we can obtain $V_0 = 0$. Therefore, we may write

$$V(x) = \frac{1}{2}V_2(x - x_0)^2. \tag{55}$$

Which we may write as

$$V(x) = \frac{\kappa x^2}{2} \tag{56}$$

if the motion is about $x_0 = 0$.

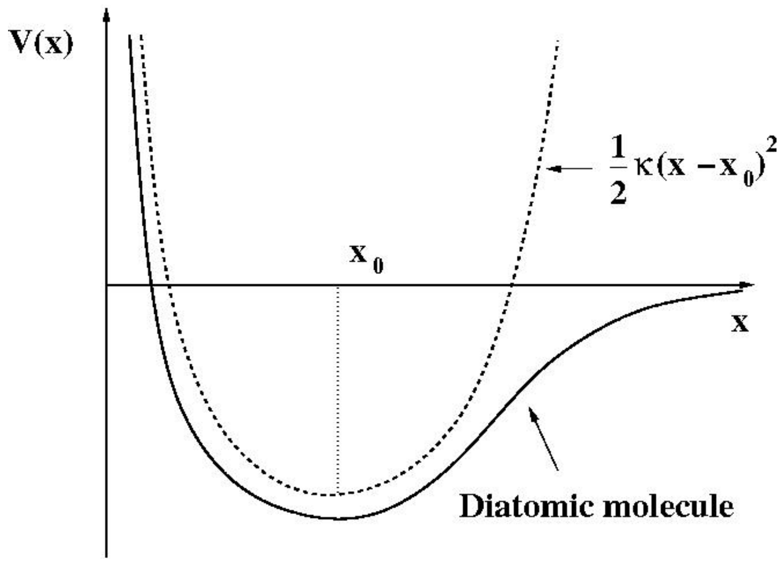

Figure 6: A simple potential representing a diatomic molecule.

5.4.1 What of the Schrödinger equation for this system?

We can write

$$\begin{aligned} E\psi &= -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{\kappa x^2}{2}\psi \\ \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} &= -\frac{2m}{\hbar^2}\left(E - \frac{\kappa x^2}{2}\right)\psi. \end{aligned} \tag{57}$$

Setting

$$\alpha^2 = \frac{m\kappa}{\hbar^2} \text{ and } \beta = \frac{2mE}{\hbar^2} \tag{58}$$

We have

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = (\alpha^2 x^2 - \beta)\psi. \tag{59}$$

Solutions to this equation, in the most general case, take the form

$$\psi(x) = Ce^{-\alpha x^2/2}. \tag{60}$$

Substituting this into the Schrödinger equation we obtain

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = -C\alpha x\, e^{-\alpha x^2/2} \tag{61}$$

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -C\alpha e^{-\alpha x^2/2} + C\alpha^2 x^2 e^{-\alpha x^2/2} \tag{62}$$

$$E\psi = -\frac{\hbar^2}{2m}[-\alpha + \alpha^2 x^2]\psi + \frac{1}{2}\kappa x^2 \psi. \tag{63}$$

If the Schrödinger equation is to hold for all values of x, then the coefficients of each power of x must be equal. Equating coefficients of x^2 we have

$$-\frac{\hbar^2}{2m}\alpha^2 + \frac{1}{2}\kappa = 0. \tag{64}$$

Therefore, $\alpha^2 = m\kappa/\hbar^2$, as defined in Equation 58. Equating the constant coefficients we have

$$E = \frac{\hbar^2}{2m}\alpha \tag{65}$$

$$= \frac{\hbar^2}{2m}\sqrt{\frac{m\kappa}{\hbar^2}} \tag{66}$$

$$= \frac{\hbar}{2}\sqrt{\frac{\kappa}{m}}. \tag{67}$$

However, $\sqrt{\kappa/m} = \omega$, the angular frequency of SHM. Therefore

$$E = \frac{\hbar\omega}{2}. \tag{68}$$

5.4.2 The uncertainty principle and the ground state energy of a quantum SHO

Consideration of the uncertainty principle demonstrates that the term $E = \hbar\omega/2$ is the minimum energy permitted for a particle constrained to move in a potential of the form $V(x) = \kappa x^2/2$. The total energy of the SHO is

$$E = KE + PE. \tag{69}$$

The minimum energy can be expressed in terms of the uncertainty in Δp and Δx, i.e.

$$E = \frac{(\Delta p)^2}{2m} + \frac{1}{2}\kappa(\Delta x)^2. \tag{70}$$

As $\kappa = m\omega^2$ we may write

$$E = \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2. \tag{71}$$

Using $\Delta p \Delta x = \hbar/2$ (note that the solution to the Schrödinger equation is a Gaussian wave function) we can re-write the energy expression as

$$E = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2} m\omega^2 (\Delta x)^2. \tag{72}$$

The minimum energy occurs at $\mathrm{d}E/\mathrm{d}(\Delta x) = 0$, i.e.

$$-\frac{\hbar^2}{4m(\Delta x)^3} + m\omega^2 \Delta x = 0, \tag{73}$$

i.e.

$$\Delta x = \sqrt{\frac{\hbar}{2m\omega}}. \tag{74}$$

Substituting this equation back into the expression for the minimum energy gives

$$\begin{aligned} E_{min} = E_0 = &= \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2} m\omega^2 (\Delta x)^2 \\ &= \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} \\ &= \frac{\hbar\omega}{2}. \end{aligned} \tag{75}$$

Therefore the ground state energy of a particle moving in a harmonic oscillator potential is the minimum energy permitted for that system. As the minimum quantum energy state $E_0 > 0$ atoms in a crystal lattice or a diatomic molecule cannot have zero energy even if cooled to absolute zero temperature. The energy of the ground state is sometimes referred to as the "zero point vibration" and is responsible for the phenomenon that, at atmospheric pressure, He^4 will never freeze, even at $T = 0$ K.

5.4.3 The exact form of the wave solution $\psi_n(x)$

When we wrote the solution to the Schrödinger equation as

$$\psi(x) = Ce^{-\alpha x^2/2} \tag{76}$$

we were actually limiting ourselves to the case $n = 0$. Note that, confusingly, the ground state of the SHO is described by $n = 0$. Before exploring the general solution in more detail, let us compute the normalisation constant for $\psi_0(x)$, i.e.

$$1 = \int_{-\infty}^{\infty} \psi_0^*(x)\psi_0(x)\mathrm{d}x \tag{77}$$

$$= \int_{-\infty}^{\infty} C^2 e^{-\alpha x^2} \mathrm{d}x \quad (78)$$

$$= 2\int_{0}^{\infty} C^2 e^{-\alpha x^2} \mathrm{d}x \quad (79)$$

$$= 2C^2 \left[\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\right] \quad (80)$$

$$C^2 = \sqrt{\frac{\alpha}{\pi}} \quad (81)$$

$$C = \left(\frac{\alpha}{\pi}\right)^{1/4}. \quad (82)$$

Therefore, the ground state is a pure Gaussian function given by

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}. \quad (83)$$

What is the form of the wave function permitted within the potential? Classically, a particle of energy E_0 will be constrained to move within $-a \leq x \leq a$ such that

$$E_0 = V_0 = \frac{1}{2}\kappa a^2. \quad (84)$$

Similarly, within the limits $|x| \leq a$ the wave function may take some general, oscillatory form. However, at $|x| > a$ the wave function must take on an exponentially declining form – recall from quantum tunneling that this is the form of the wave function permitted for $E < V_0$ (Figure 7).

5.4.4 The correspondence principle and the quantum oscillator

We have constructed a quantum description of a SHO but Newton's laws still provide an adequate description for the motion of a mass on a spring. To see how the quantum model transforms into the classical model we can consider the probability of observing a particle at a particular location in a simple harmonic system. This is equivalent to forming $P(x) = \psi^*\psi$ and values of $P_n(x)$ are displayed in Figure 8.

In a classical system, we are most likely to observe the oscillating particle where it spends most of the time. This probability, $P_c \propto 1/V_x$, where V_x is the transverse velocity of the particle. We can understand the form of $P_c(x)$ by noting that the particle is stationary at $x = \pm a$ and is moving most rapidly at $x = 0$. Therefore, there is a considerable difference between the classical and quantum models for $n = 0$. However, as n tends to some large number the form of $P_n(x)$ tends to $P_c(x)$ exactly as expected from the correspondence principle.

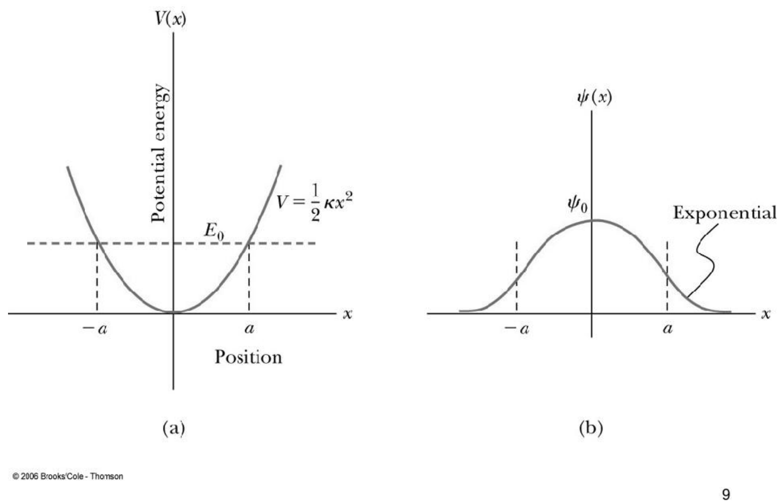

Figure 7: The form of the wave function permitted in a simple harmonic potential.

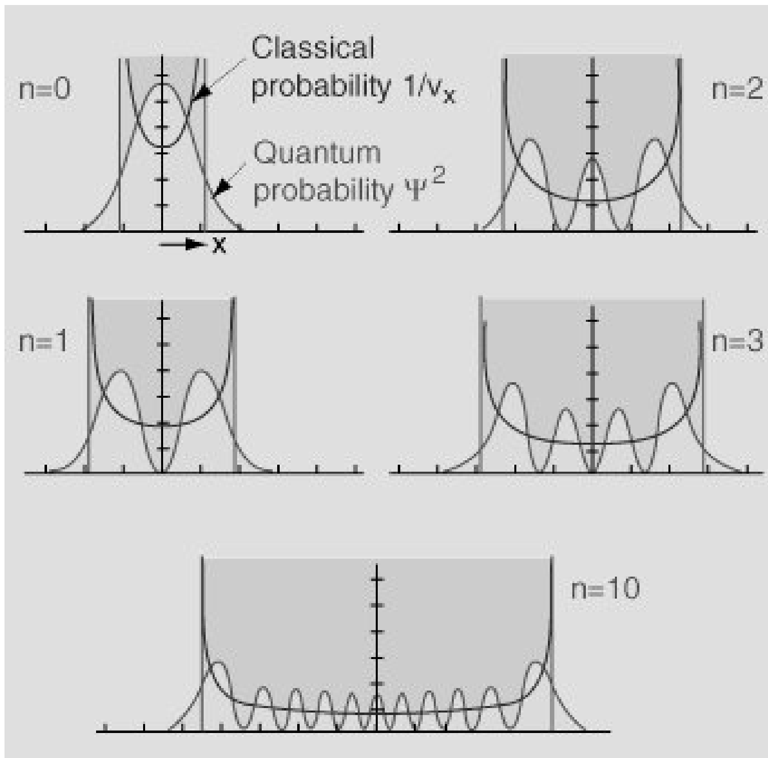

Figure 8: The relationship between classical and quantum probability for a simple harmonic oscillator.