Quantum Mechanics

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Spring 2005

Chapter 4

Solutions of Time-Independent Schrödinger Equations

4.1 The Zero Potential

This is the case where $V(x) = 0$ for all x.

Our Time-Independent Schrödinger Equation is

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

The most general solution for this second order linear ordinary differential equation is of the form

$$\psi(x) = A_1 \sin\frac{\sqrt{2mE}}{\hbar}x + A_2 \cos\frac{\sqrt{2mE}}{\hbar}x = C_1 e^{ikx} + C_2 e^{-ikx};$$

where A_1, A_2, C_1, and C_2 are arbitrary constants, and $k = \frac{\sqrt{2mE}}{\hbar}$.

On the other hand, we always have

$$\phi(t) = e^{-iEt/\hbar} = e^{-ih\nu t/(h/2\pi)} = e^{-i2\pi\nu t} = e^{-i\omega t}$$

for time dependence.

Therefore, the full time-dependent wavefunction is

$$\Psi(x,t) = \psi(x)\phi(t) = \left(C_1 e^{ikx} + C_2 e^{-ikx}\right)e^{-i\omega t} = C_1 e^{i(kx-\omega t)} + C_2 e^{-i(kx+\omega t)}.$$

Let us take

$$\Psi(x,t) = C_1 e^{i(kx-\omega t)} \left(= C_1 e^{ikx} e^{-iEt/\hbar}\right).$$

Then,

$$\overline{P} = \langle P \rangle = \int_{-\infty}^{+\infty} \Psi^* P \Psi dx = \int_{-\infty}^{+\infty} C_1^* e^{-ikx} e^{iEt/\hbar} (-i\hbar) \frac{\partial}{\partial x} C_1 e^{ikx} e^{-iEt/\hbar} dx$$

$$= \int_{-\infty}^{+\infty} C_1^* e^{-ikx} e^{iEt/\hbar} (-i\hbar)(ik) C_1 e^{ikx} e^{-iEt/\hbar} dx = \left(\int_{-\infty}^{+\infty} \Psi^* \Psi dx\right) = \hbar k \int_{-\infty}^{+\infty} \psi^* \psi dx$$

$$= \hbar k = \frac{h}{2\pi} \cdot \frac{2mE}{\hbar} = \sqrt{2mE}.$$

This makes sense as

$$\frac{P^2}{2m} = E \Longrightarrow P = \sqrt{2mE}$$

classically.

The computation above serves as yet another consistency checking device.

4.2 The Step Potential ($E < V_0$)

We now consider a step potential given by

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

for $E < V_0$.

In Newtonian (classical) mechnics, the particle can not enter the region $(0, \infty)$. We have

$$E = K.E. + P.E. = K.E. + V_0 \text{ in } (0,\infty) \Longrightarrow K.E. = E - V_0 < 0.$$

This does not make any sense of any kind classically. Is this also the case in quantum mechanics? Let us just plunge in and solve it!

The time-independent Schrödinger Equation is

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

In our case, we have the following.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad x \leq 0 \tag{4.1}$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \qquad x > 0 \tag{4.2}$$

Equation 4.1 is that for a free particle. Therefore, the general solution is

$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x};$ where $k_1 = \dfrac{\sqrt{2mE}}{\hbar}$, and A and B are arbitrary constants.

On the other hand, equation 4.2 can be rewritten as follows.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = (E-V_0)\psi(x) \Longleftrightarrow \frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = (V_0-E)\psi(x) \Longleftrightarrow \frac{d^2\psi(x)}{dx^2} = \frac{2m(E-V_0)}{\hbar^2}\psi(x)$$

The general solution for $x > 0$ is

$\psi(x) = Ce^{k_2x}+De^{-k_2x};$ where $k_2 = \dfrac{2m(V_0-E)}{\hbar}$, and C and D are arbitrary constants.

Note that $V_0 - E$ is positive in this region.

As stated above, these are indeed the solution, or the (most) general solution, since we have a linear second order ordinary differential equations.

We have

$$\begin{cases} \psi(x) = Ae^{ik_1x} + Be^{-ik_1x} & (k_1 = \frac{\sqrt{2mE}}{\hbar}) & x \leq 0 \\ \psi(x) = Ce^{k_2x} + De^{-k_2x} & (k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}) & x > 0 \end{cases} .$$

Recall the conditions on $(\psi, \frac{d\psi}{dx})$.

1. Finite
2. Single-valued
3. Continuous

We will determine A, B, C, and D using these conditions.

Let us begin with the region $x > 0$. In this region,

$$\psi(x) = Ce^{k_2 x} + De^{-k_2 x}; \text{ where } k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}.$$

Therefore,

$$\begin{aligned}\psi^*(x)\psi(x) &= \left(C^* e^{k_2 x} + D^* e^{-k_2 x}\right)\left(Ce^{k_2 x} + De^{-k_2 x}\right) \\ &= |C|^2 e^{2k_2 x} + \overbrace{D^* C + C^* D}^{2ReC^* D} + |D|^2 e^{-2k_2 x}.\end{aligned}$$

Since the wavefunction has to be normalizable, it has to satisfy the finiteness condition

$$\int_{-\infty}^{+\infty} \psi^*(x)\psi(x)dx = \int_{-\infty}^{+\infty} |\psi(x)|^2 dx < \infty.$$

Noting that this ψ is the wavefuntion only in the region $x > 0$, we actually need

$$\int_0^{+\infty} |\psi(x)|^2 dx < \infty.$$

Hence, we have to have

$$C = 0.$$

At this point, we have

$$\begin{cases} \psi(x) = Ae^{ik_1 x} + Be^{-ik_1 x} & k_1 = \frac{\sqrt{2mE}}{\hbar} & x \le 0 \\ \psi(x) = De^{-k_2 x} & (k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}) & x > 0 \end{cases}.$$

Next, we will use the continuity condition on $\psi(x)$ and $\frac{d\psi(x)}{dx}$.
Continuity of $\psi(x)$ at $x = 0$ gives

$$De^{-k_2 \cdot 0} = Ae^{ik_1 \cdot 0} + Be^{-ik_1 \cdot 0} \Longrightarrow D = A + B.$$

Since the first derivative is

$$\begin{cases} \frac{d\psi(x)}{dx} = A(ik_1)e^{ik_1 x} + B(-ik_1)e^{-ik_1 x} & k_1 = \frac{\sqrt{2mE}}{\hbar} & x \le 0 \\ \frac{d\psi(x)}{dx} = D(-k_2)e^{-k_2 x} & (k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}) & x > 0 \end{cases},$$

continuity of $\frac{d\psi(x)}{dx}$ at $x = 0$ gives

$$-k_2 D e^{-k_2 \cdot 0} = ik_1 A e^{ik_1 \cdot 0} - ik_1 B e^{-ik_1 \cdot 0} \Longrightarrow -k_2 D = ik_1(A - B) \Longrightarrow \frac{-k_2}{ik_1} D = A - B.$$

We now have a simultaneous equation

$$\left\{ \begin{array}{rcl} \frac{ik_2}{k_1} D & = & A - B \\ D & = & A + B \end{array} \right.$$

for A, B, and D with the solution

$$\begin{array}{rcl} A & = & \frac{1}{2}\left(1 + \frac{ik_2}{k_1}\right) D \\ B & = & \frac{1}{2}\left(1 - \frac{ik_2}{k_1}\right) D \end{array}.$$

This gives

$$\psi(x) = \left\{ \begin{array}{cl} \frac{D}{2}(1 + ik_2/k_1)e^{ik_1 x} + \frac{D}{2}(1 - ik_2/k_1)e^{-ik_1 x} & x \leq 0 \\ De^{-k_2 x} & x > 0 \end{array} \right. .$$

So, the full solution is

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

$$= \left\{ \begin{array}{cl} \frac{D}{2}(1 + ik_2/k_1)e^{i(k_1 x - Et/\hbar)} + \frac{D}{2}(1 - ik_2/k_1)e^{-i(k_1 x + Et/\hbar)} & x \leq 0 \\ De^{-k_2 x}e^{-iEt/\hbar} & x > 0 \end{array} \right. .$$

Recall that

$$e^{-iEt/\hbar} = e^{-i\omega t}.$$

This is because

$$Et/\hbar = h\nu t/\hbar = h\nu t/(\frac{h}{2\pi}) = 2\pi\nu t = \omega t.$$

Therefore, in the region $x \leq 0$,

$$\Psi(x, t) = Ae^{i(k_1 x - \omega t)} + Be^{i(-k_1 x - \omega t)}.$$

Note that

$$Ae^{i(k_1x-\omega t)}$$

is traveling to the right while

$$Be^{i(-k_1x-\omega t)}$$

is traveling to the left.

In other words,

$$Ae^{i(k_1x-\omega t)}$$

is the incident wave, incident on the step form the left, while

$$Be^{i(-k_1x-\omega t)}$$

is the wave reflected by the step.

What is the reflection coefficient? Since the reflection coefficient is the ratio of the amplitude of the reflected wave and the amplitude of the indident wave, we have

$$\text{the reflection coefficient} = \frac{\text{the amplitude of the reflected wave}}{\text{the amplitude of the incident wave}}$$

$$= \frac{|Be^{i(-k_1x-\omega t)}|^2}{|Ae^{i(k_1x-\omega t)}|^2} = \frac{|B|^2|e^{i(-k_1x-\omega t)}|^2}{|A|^2|e^{i(k_1x-\omega t)}|^2} = \frac{|B|^2}{|A|^2} = \frac{B^*B}{A^*A} = \frac{\frac{D^*}{2}\left(1-i\frac{k_2}{k_1}\right)^*\frac{D}{2}\left(1-i\frac{k_2}{k_1}\right)}{\frac{D^*}{2}\left(1+i\frac{k_2}{k_1}\right)^*\frac{D}{2}\left(1+i\frac{k_2}{k_1}\right)}$$

$$= \frac{\left(1+i\frac{k_2}{k_1}\right)\left(1-i\frac{k_2}{k_1}\right)}{\left(1-i\frac{k_2}{k_1}\right)\left(1+i\frac{k_2}{k_1}\right)} = 1$$

And, we have a total reflection.

Indeed, we have a standing wave in the region $x \le 0$. To see this, plug $e^{ik_1x} = \cos k_1x + i\sin k_1x$ into

$$\psi(x) = \begin{cases} \frac{D}{2}\left[(1+ik_2/k_1)e^{ik_1x} + (1-ik_2/k_1)e^{-ik_1x}\right] & x \le 0 \\ De^{-k_2x} & x > 0 \end{cases}$$

to obtain

$$\psi(x) = \begin{cases} D\cos k_1x - D\frac{k_2}{k_1}\sin k_1x & x \le 0 \\ De^{-k_2x} & x > 0 \end{cases}.$$

So, for $x \le 0$,

$$\Psi(x,t) = D\left(\cos k_1x - \frac{k_2}{k_1}\sin k_1x\right)e^{-iEt/\hbar}.$$

Remember the following from high school math,

$$\alpha \cos kx - \beta \sin kx = \left(\frac{\alpha}{\sqrt{\alpha^2+\beta^2}} \cos kx - \frac{\beta}{\sqrt{\alpha^2+\beta^2}} \sin kx \right) \sqrt{\alpha^2+\beta^2} = \cos(kx+\theta);$$

where θ is such that

$$\cos\theta = \frac{\alpha}{\sqrt{\alpha^2+\beta^2}} \text{ and } \sin\theta = \frac{\beta}{\sqrt{\alpha^2+\beta^2}}.$$

Therefore, the nodes do not move, and we indeed have a standing wave.

Now, in the region $x > 0$,

$$\Psi^*(x,t)\Psi(x,t) = D^* D e^{-2k_2 x}.$$

While

$$\lim_{x\to\infty} \Psi^*\Psi = 0,$$

$$\Psi^*\Psi \neq 0$$

for $\forall x > 0$. This means that the probability of finding the particle to the right of the step is not zero even if the total energy E is smaller than the step height V_0. This phenomenon is definitely nonclassical and is known as "barrier penetration".

4.3 The Step Potential ($E > V_0$)

We will now consider the case where the total enrgy E is greater than the step height.

Classically, we have the following.

1. Not a total reflection
2. Has to be a total penetration into $(0, \infty)$

But, quantum mechanically, the Schrödinger Equation predicts the following.

1. Not a total reflection (agreement with the classical theory)
2. Has to be a total penetration into $(0, \infty)$ (disagreement)

Let us see how it works.

As usual, $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$, and the Time-Independent Schrödinger Equation is

$$\begin{cases} \frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} &= E\psi(x) \quad x<0 \\ \frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} &= (E-V_0)\psi(x) \quad x>0 \end{cases}$$

Since $E - V_0 > 0$ this time, the two equations are basically the same. They are both free particles, and the solutions are

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x<0 \\ Ce^{ik_2x} + De^{-ik_2x} & x>0 \end{cases};$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$.

Suppose the particle is in the region $x < 0$ or $(-\infty, 0)$ at $t = 0$. In other words, the particle is incident on the step from the left. Then, since the wave is travelling to the right in the region $(0,\infty)$, we should set $D = 0$. This is simply because $e^{-ik_2x}e^{-iEt/\hbar}$ is a wave travelling to the left.

Imposing the continuity condition on ψ and $\frac{d\psi}{dx}$ at $x = 0$, we can express the constants B and C in terms of A as follows.

$$\left\{ \begin{array}{rcl} \psi(x)|_{x=0-} &=& \psi(x)|_{x=0+} \\ \left.\frac{d\psi(x)}{dx}\right|_{x=0-} &=& \left.\frac{d\psi(x)}{dx}\right|_{x=0+} \end{array} \right\} \Longrightarrow \left\{ \begin{array}{rcl} A+B &=& C \\ k_1(A-B) &=& k_2C \end{array} \right. \Longrightarrow \left\{ \begin{array}{rcl} B &=& A\frac{k_1-k_2}{k_1+k_2} \\ C &=& A\frac{2k_1}{k_1+k_2} \end{array} \right.$$

Therefoere,

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

The reflection coefficient R is given by

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

Since the transmission coefficient T is related to R via $R + T = 1$,

$$T = 1 - R = 1 - \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 = \frac{(k_1+k_2+k_1-k_2)(k_1+k_2-k_1+k_2)}{(k_1+k_2)^2} = \frac{4k_1k_2}{(k_1+k_2)^2}.$$

As advertised, we do not have a total reflection, and we do not have a total penetration into $(0,\infty)$, either.

We now solve the same problem for a wave incident on the potential boundary at $x = 0$ from the right. In other words, the particle is in the region $(0, \infty)$ at $t = 0$ and traveling to the left.

Our general solution is

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x} & x < 0 \\ Ce^{ik_2 x} + De^{-ik_2 x} & x > 0 \end{cases};$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$.

Since there is no boundary to reflect the wave in the region $(-\infty, 0)$, the wave should be travelling to the left in this region. We set $A = 0$.

$$\psi(x) = \begin{cases} Be^{-ik_1 x} & x < 0 \\ Ce^{ik_2 x} + De^{-ik_2 x} & x > 0 \end{cases}$$

The first derivative with respect to x is

$$\psi(x) = \begin{cases} -ik_1 Be^{-ik_1 x} & x < 0 \\ ik_2 Ce^{ik_2 x} + (-ik_2)De^{-ik_2 x} & x > 0 \end{cases}.$$

Imposing the continuity condition on $\psi(x)$ and $\frac{d\psi(x)}{dx}$ at $x = 0$, we get

$$\begin{cases} B &= C + D \\ -ik_1 B &= ik_2(C - D) \end{cases} \Longrightarrow \begin{cases} C + D &= B \\ C - D &= -\frac{k_1}{k_2}B \end{cases} \Longrightarrow \begin{cases} C &= \frac{k_2-k_1}{2k_2}B \\ D &= \frac{k_2+k_1}{2k_2}B \end{cases}.$$

What are the reflection coefficient and the transmission coefficient in this case?

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

and

$$T = 1 - R = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

Note that these are the same as before when we computed R and T for the particle moving in from the left.

Incidentally, $B \neq 0$ can be proved on purely mathematical gorunds as follows.

If $B = 0$,

$$\psi(x) = \begin{cases} Ae^{ik_1 x} & x < 0 \\ Ce^{ik_2 x} & x > 0 \end{cases} \Longrightarrow \begin{cases} A & = & C \\ k_1 A & = & k_2 C \end{cases} .$$

But, it is obvious that this can not be solved for A and C unless we accept $A = C = 0$ which is physically meaningless. Hence, $B \neq 0$ on this ground.

4.4 The Barrier Potential ($E < V_0$)

The potential $V(x)$ is V_0 in the region $(0, a)$ and 0 elsewhere.

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

Our Time-Independent Schrödinger Equation is

$$\psi(x) = \begin{cases} Ae^{ik_1 x} & + & Be^{-ik_1 x} & x < 0 \\ Fe^{-k_2 x} & + & Ge^{k_2 x} & 0 < x < a \\ Ce^{ik_1 x} & + & De^{-ik_1 x} & x > a \end{cases} ;$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$.
Assuming $x < 0$ at $t = 0$, $D = 0$.
On the other hand, our boundary conditions are

$$\begin{cases} \psi(x)|_{x=0-} & = & \psi(x)|_{x=0+} \\ \psi(x)|_{x=a-} & = & \psi(x)|_{x=a+} \\ \left.\frac{d\psi(x)}{dx}\right|_{x=0-} & = & \left.\frac{d\psi(x)}{dx}\right|_{x=0+} \\ \left.\frac{d\psi(x)}{dx}\right|_{x=a-} & = & \left.\frac{d\psi(x)}{dx}\right|_{x=a+} \end{cases} .$$

We have the above four equations and the five unknowns A, B, C, F, and G. But, we also have a normalization condition. So, we can solve for the five unknowns.

As it turned out, $C \neq 0$, and the probability density $\Psi^*(x,t)\Psi^*(x,t) = \psi^*(x)\psi(x)$ has a (nonzero) tail in the region $x > a$. Of course, it is nonzero also inside the barrier.
Therefore, we have both *barrier penetration* and *tunneling*.

4.5 The Infinite Square Well Potential

The potential is given by

$$V(x) = \begin{cases} \infty & |x| > \frac{a}{2} \\ 0 & |x| < \frac{a}{2} \end{cases} ,$$

and we get, as we have already seen,

$$\psi(x) = \begin{cases} 0 & |x| > \frac{a}{2} \\ A\sin kx + B\cos kx & |x| < \frac{a}{2} \end{cases};$$

where $k = \frac{\sqrt{2mE}}{\hbar}$. As usual, the full wavefunction is

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

It turned out the continuity condition of the first derivative is too restrictive for this system as the potential blows up to ∞ unlike any known physical system. The continuity condition on $\psi(x)$ at $|x| = \frac{a}{2}$ gives

$$\begin{cases} A\sin\frac{ka}{2} + B\cos\frac{ka}{2} = 0 \\ -A\sin\frac{ka}{2} + B\cos\frac{ka}{2} = 0 \end{cases} \Longrightarrow \begin{cases} 2B\cos\frac{ka}{2} = 0 \\ 2A\sin\frac{ka}{2} = 0 \end{cases} \Longrightarrow \begin{cases} A = 0 \ \underline{\text{and}} \ \cos\frac{ka}{2} = 0 \\ B = 0 \ \underline{\text{and}} \ \sin\frac{ka}{2} = 0 \end{cases}.$$

Therefore,

$$\begin{cases} \psi(x) = B\cos kx \quad \text{where} \quad \cos\frac{ka}{2} = 0 \\ \qquad \underline{\text{or}} \\ \psi(x) = A\sin kx \quad \text{where} \quad \sin\frac{ka}{2} = 0 \end{cases}.$$

We have two families of solutions.

$$\begin{cases} \psi_n(x) = B_n\cos k_nx \quad \text{where} \quad k_n = \frac{n\pi}{a} \quad n = 1,3,5,\ldots \\ \psi_n(x) = A_n\sin k_nx \quad \text{where} \quad k_n = \frac{n\pi}{a} \quad n = 2,4,6,\ldots \end{cases}.$$

Note that n is a positive integer in both cases. This is becasue negative n's give redundant solutions and $n = 0$ gives a physically meaningless solution. Indeed,

$$n = 0 \Longrightarrow \psi_0(x) = A_0\sin 0 = 0.$$

Since $k_n = \sqrt{2mE_n}/\hbar$, the total energy E_n can only take discrete values.

$$k_n = \frac{\sqrt{2mE_n}}{\hbar} \Longrightarrow 2mE_n = \hbar^2k_n^2 \Longrightarrow E_n = \frac{\hbar^2k_n^2}{2m} = \frac{\pi^2\hbar^2n^2}{2ma^2} \quad n = 1,2,3,4,5,\ldots$$

Note that $E_n \propto n^2$ and the spacing between neighboring energy levels

$$E_{n+1} - E_n = \frac{\pi^2\hbar^2(n+1)^2}{2ma^2} - \frac{\pi^2\hbar^2n^2}{2ma^2} = \frac{\pi^2\hbar^2(2n+1)}{2ma^2}$$

is proportional to $2n+1$. This is the reason for the widening of the gap as $n \to \infty$. More significant implication of this is that the particle can not have zero total energy. Indeed, the lowest energy level

$$E_1 = \frac{\pi^2\hbar^2}{2ka^2} > 0.$$

This is one reason why absolute zero degree temperature can not be achieved. While the infinite square well potential is a mathematical idealization, it approximates the potential well experienced by atoms or nuclei in a crystal for example.

Another type of bound system frequently encountered in nature is a diatomic molecule.

4.6 The Simple Harmonic Oscillator Potential

Consider a typical spring encountered in high school physics with a spring constant k such that the restoring force F is given by $F = -kx$ for the displacement x from the equilibrium position. For no other reason than convention, we will use c instead of k for the spring constant.

Since
$$V(x) = \frac{1}{2}cx^2,$$
the Time-Independent Schrödinger Equation is
$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{c}{2}x^2\psi(x) = E\psi(x).$$
We will need some fancy footwork to solve this equation. As it turns out, it is convenient to introduce a new variable ν analogously to the classical theory. Hence,
$$\nu = \frac{1}{2\pi}\sqrt{\frac{c}{m}}.$$
After substituting $c = (2\pi)^2\nu^2 m$ into the equation and dividing through by $\frac{-\hbar^2}{2m}$, we get
$$\frac{d^2\psi}{dx^2} + \left[\frac{2mE}{\hbar^2} - \left(\frac{2\pi m\nu}{\hbar}\right)^2 x^2\right]\psi = 0.$$
Now, let $\alpha = 2\pi m\nu/\hbar$ and $\beta = 2mE/\hbar^2$ to simplify the equation to
$$\frac{d^2\psi}{dx^2} + (\beta - \alpha^2x^2)\psi = 0.$$
Here are further manipulatinos.
$$u = \sqrt{\alpha}x = \left[\frac{2\pi m}{\hbar 2\pi}(\frac{c}{m})^{1/2}\right]^{1/2} x = \frac{(cm)^{1/4}}{\hbar^{1/2}}x$$

$$\frac{d\psi}{dx} = \frac{d\psi}{du}\frac{du}{dx} = \sqrt{\alpha}\frac{d\psi}{du}$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \frac{d(\frac{d\psi}{dx})}{dx} = \frac{d(\sqrt{\alpha}\frac{d\psi}{du})}{dx} = \frac{du}{dx}\frac{d}{du}\left(\sqrt{\alpha}\frac{d\psi}{du}\right) = \sqrt{\alpha}\sqrt{\alpha}\frac{d}{du}\left(\frac{d\psi}{du}\right) = \alpha\frac{d^2\psi}{du^2}$$

You may be more comfortable with the following.

$$du = \sqrt{\alpha}dx \quad \Longrightarrow \quad dx = \frac{1}{\sqrt{\alpha}}du$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{\frac{1}{\sqrt{\alpha}}du}\left(\frac{d\psi}{\frac{1}{\sqrt{\alpha}}du}\right) = \alpha\frac{d^2\psi}{du^2}$$

Either way is fine, and we now have

$$\frac{d^2\psi}{dx^2} + (\beta - \alpha^2 x^2)\psi = \alpha\frac{d^2\psi}{du^2} + (\beta - \alpha u^2)\psi = 0 \quad \Longrightarrow \quad \frac{d^2\psi}{du^2} + \left(\frac{\beta}{\alpha} - u^2\right)\psi = 0.$$

Here comes a very inexact argument.

As $|u| \to \infty$, the differential equation behaves like

$$\frac{d^2\psi}{du^2} - u^2\psi = 0$$

or

$$\frac{d^2\psi}{du^2} = u^2\psi$$

since β/α is a constant.
The (mathematical) general solution of this differential equation is

$$\psi = Ae^{-u^2/2} + Be^{u^2/2}.$$

But, we have to set

$$B = 0$$

to satisfy the finiteness condition. So,

$$\psi(u) = Ae^{-u^2/2} \qquad |u| \to \infty.$$

We will look for a solution of the form

$$\psi(u) = Ae^{-u^2/2}H(u);$$

where $H(u)$ must be slowly varying in comparison to $e^{-u^2/2}$.
Compute $\frac{d^2\psi(u)}{du^2}$, then plug it back into the equation

$$\frac{d^2\psi(u)}{du^2} + \left(\frac{\beta}{\alpha} - u^2\right)\psi(u) = 0$$

to obtain

$$\frac{d^2H}{du^2} - 2u\frac{dH}{du} + \left(\frac{\beta}{\alpha} - 1\right)H = 0.$$

We will try a power series solution for $H(u)$.
Let

$$H(u) = \sum_{l=0}^{\infty} a_l \cdot u^l = a_0 + a_1 u + a_2 u^2 + a_3 u^3 + \cdots .$$

Then,

$$u\frac{dH(u)}{du} = (a_1 + 2a_2 u + 3a_3 u^2 + 4a_4 u^3 + \cdots)u = \left(\sum_{l=0}^{\infty}(l+1)a_{l+1}u^l\right) \cdot u$$

$$= \sum_{l=0}^{\infty}(l+1)a_{l+1}u^{l+1} = \sum_{l=1}^{\infty} l a_l u^l$$

and

$$\frac{d^2H(u)}{du^2} = 2a_2 + 3 \cdot 2a_3 u + 3 \cdot 4a_4 u^2 + \cdots = \sum_{l=0}^{\infty}(l+1)(l+2)a_{l+2}u^l.$$

Plugging the above into

$$\frac{d^2H}{du^2} - 2u\frac{dH}{du} + \left(\frac{\beta}{\alpha} - 1\right)H = 0$$

gives us

$$\sum_{l=0}^{\infty}(l+1)(l+2)a_{l+2}u^l - 2\sum_{l=0}^{\infty} l a_l u^l + \left(\frac{\beta}{\alpha} - 1\right)\sum_{l=0}^{\infty} a_l u^l = 0$$

or

$$\sum_{l=0}^{\infty}\left[(l+1)(l+2)a_{l+2} - 2la_l + \left(\frac{\beta}{\alpha} - 1\right)a_l\right]u^l = 0.$$

For a power series to be zero, each term has to be zero; that is to say all the coefficients have to be zero.
We now have the following recursion relation.

$$a_{l+2} = -\frac{(\beta/\alpha - 1 - 2l)}{(l+1)(l+2)}a_l$$

The general solution is of the following form.

$$H(u) = a_0\left(1 + \frac{a_2}{a_0}u^2 + \frac{a_4a_2}{a_2a_0}u^4 + \frac{a_6a_4a_2}{a_4a_2a_0}u^6 + \cdots\right) + a_1\left(u + \frac{a_3}{a_1}u^3 + \frac{a_5a_3}{a_3a_1}u^5 + \frac{a_7a_5a_3}{a_5a_3a_1}u^7 + \cdots\right)$$

As $|u| \to \infty$, $\frac{a_{l+2}}{a_l} \to \frac{2}{l}$, and $H(u)$ behaves like

$$H(u) = a_0Ke^{u^2} + a_1K'ue^{u^2}.$$

So, $e^{-u^2/2}H(u)$ behaves like

$$a_0Ke^{u^2/2} + a_1K'ue^{u^2/2} \qquad \text{as} \quad |u| \to \infty$$

Therefore, $H(u)$ has to terminate after some n. We have to set $\beta/\alpha = 2n + 1$ for $n = 0, 1, 2, 3, 4, 5, \ldots$.

When $\beta/\alpha = 2n + 1$ we get a Hermite polynomial denoted by $H_n(u)$. This gives us a series of eigenfunctions

$$\psi_n(u) = A_ne^{-u^2/2}H_n(u).$$

The first six functions look like this.

$$\begin{array}{rl}
n = 0 & \psi_0 = A_0e^{-u^2/2} \\
1 & \psi_1 = A_1ue^{-u^2/2} \\
2 & \psi_2 = A_2(1 - 2u^2)e^{-u^2/2} \\
3 & \psi_3 = A_3(3u - 2u^3)e^{-u^2/2} \\
4 & \psi_4 = A_4(3 - 12u^2 + 4u^4)e^{-u^2/2} \\
5 & \psi_5 = A_5(15u - 20u^3 + 4u^5)e^{-u^2/2}
\end{array}$$

Now recall that $u = \sqrt{\alpha}x$, $\alpha = 2\pi m\nu/\hbar$, and $\beta = 2mE/\hbar^2$.

$$\beta/\alpha = \frac{2mE/\hbar^2}{2\pi m\nu/\hbar} = \frac{E}{\hbar\pi\nu} = \frac{E}{\frac{h}{2\pi}\cdot\pi\nu} = \frac{2E}{h\nu}$$

Setting this equal to $2n + 1$,

$$\beta/\alpha = 2n+1 \Longrightarrow \frac{2E_n}{h\nu} = 2n+1 \Longrightarrow E_n = \left(n + \frac{1}{2}\right)h\nu \qquad n = 0, 1, 2, 3, 4, 5, \ldots.$$

Recall that

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

Therefore, if the force constant c and the mass m are known, we know the energy levels of this harmonic oscillator.

These are the two important facts about the simple harmonic oscillator.

1. The energy levels are equally spaced. This is markedly different from the infinite square well. This means many higher energy levles can be achieved more easily.

2. The lowest energy posssible is not zero but $E_0 = \frac{1}{2}h\nu$ for $n = 0$. Since vibrations of diatomic molecules can be closely approximated by the simple harmonic oscillator, this is another reason why the absolute zero degree temperature can not be achieved.

When a molecule drops from a higher energy level to a lower level, a photon carrying that much energy is released. On the other hand, a molecule moves to a higher energy level if it absorbs a photon carrying the energy corresponding to the difference between the two levels. These phenomena are called *emission* and *absorption* respectively.

Finally, the above emission and absorption typically occur in the microwave region. While not a diatomic molecule, the excited vibration of water molecules in food is responsible for the cooking done with a microwave oven. This is why we call it a microwave oven to begin with.