4.7: Simple Harmonic Oscillator

The classical Hamiltonian of a simple harmonic oscillator is

$$H = \frac{p^{\,2}}{2\,m} + \frac{1}{2}\,K\,x^{\,2}, \tag{4.7.1}$$

where $K > 0$ is the so-called force constant of the oscillator. Assuming that the quantum mechanical Hamiltonian has the same form as the classical Hamiltonian, the time-independent Schrödinger equation for a particle of mass m and energy E moving in a simple harmonic potential becomes

$$\frac{d^{\,2}\psi}{dx^{\,2}} = \frac{2\,m}{\hbar^{\,2}}\left(\frac{1}{2}\,K\,x^{\,2} - E\right)\psi. \tag{4.7.2}$$

Let $\omega = \sqrt{K/m}$, where ω is the oscillator's classical angular frequency of oscillation. Furthermore, let

$$y = \sqrt{\frac{m\,\omega}{\hbar}}\,x, \tag{4.7.3}$$

and

$$\epsilon = \frac{2\,E}{\hbar\,\omega}. \tag{4.7.4}$$

Equation ([e5.90]) reduces to

$$\frac{d^{\,2}\psi}{dy^{\,2}} - (y^{\,2} - \epsilon)\,\psi = 0. \tag{4.7.5}$$

We need to find solutions to the previous equation which are bounded at infinity: that is, solutions which satisfy the boundary condition $\psi \to 0$ as $|y| \to \infty$.

Consider the behavior of the solution to Equation ([e5.93]) in the limit $|y| \gg 1$. As is easily seen, in this limit the equation simplifies somewhat to give

$$\frac{d^{\,2}\psi}{dy^{\,2}} - y^{\,2}\,\psi \simeq 0. \tag{4.7.6}$$

The approximate solutions to the previous equation are

$$\psi(y) \simeq A(y)\,{\rm e}^{\pm y^{\,2}/2}, \tag{4.7.7}$$

where $A(y)$ is a relatively slowly varying function of y. Clearly, if $\psi(y)$ is to remain bounded as $|y| \to \infty$ then we must chose the exponentially decaying solution. This suggests that we should write

$$\psi(y) = h(y)\,{\rm e}^{-y^{\,2}/2}, \tag{4.7.8}$$

where we would expect $h(y)$ to be an algebraic, rather than an exponential, function of y.

Substituting Equation ([e5.96]) into Equation ([e5.93]), we obtain

$$\frac{d^{\,2}h}{dy^{\,2}} - 2\,y\,\frac{dh}{dy} + (\epsilon - 1)\,h = 0. \tag{4.7.9}$$

Let us attempt a power-law solution of the form

$$h(y) = \sum_{i=0,\infty} c_i\,y^{\,i}. \tag{4.7.10}$$

Inserting this test solution into Equation ([e5.97]), and equating the coefficients of $y^{\,i}$, we obtain the recursion relation

$$c_{i+2} = \frac{(2\,i - \epsilon + 1)}{(i+1)\,(i+2)}\,c_i. \tag{4.7.11}$$

Consider the behavior of $h(y)$ in the limit $|y|\rightarrow\infty$. The previous recursion relation simplifies to

$$c_{i+2}\simeq\frac{2}{i}\,c_i. \tag{4.7.12}$$

Hence, at large $|y|$, when the higher powers of y dominate, we have

$$h(y)\sim C\sum_j\frac{y^{\,2j}}{j!}\sim C\,\mathrm{e}^{\,y^{\,2}}. \tag{4.7.13}$$

It follows that $\psi(y)=h(y)\,\exp(-y^{\,2}/2)$ varies as $\exp(\,y^{\,2}/2)$ as $|y|\rightarrow\infty$. This behavior is unacceptable, because it does not satisfy the boundary condition $\psi\rightarrow 0$ as $|y|\rightarrow\infty$. The only way in which we can prevent ψ from blowing up as $|y|\rightarrow\infty$ is to demand that the power series ([e5.98]) terminate at some finite value of i. This implies, from the recursion relation ([e5.99]), that

$$\epsilon=2\,n+1, \tag{4.7.14}$$

where n is a non-negative integer. Note that the number of terms in the power series ([e5.98]) is $n+1$. Finally, using Equation ([e5.92]), we obtain

$$E=(n+1/2)\,\hbar\,\omega, \tag{4.7.15}$$

for $n=0,1,2,\cdots$.

Hence, we conclude that a particle moving in a harmonic potential has quantized energy levels that are equally spaced. The spacing between successive energy levels is $\hbar\,\omega$, where ω is the classical oscillation frequency. Furthermore, the lowest energy state ($n=0$) possesses the finite energy $(1/2)\,\hbar\,\omega$. This is sometimes called *zero-point energy*. It is easily demonstrated that the (normalized) wavefunction of the lowest energy state takes the form

$$\psi_0(x)=\frac{\mathrm{e}^{-x^2/2d^2}}{\pi^{1/4}\sqrt{d}} \tag{4.7.16}$$

Let $\psi_n(x)$ be an energy eigenstate of the harmonic oscillator corresponding to the eigenvalue

$$E_n=(n+1/2)\,\hbar\,\omega. \tag{4.7.17}$$

Assuming that the ψ_n are properly normalized (and real), we have

$$\int_{-\infty}^{\infty}\psi_n\,\psi_m\,dx=\delta_{nm}. \tag{4.7.18}$$

Now, Equation ([e5.93]) can be written

$$\left(-\frac{d^{\,2}}{dy^{\,2}}+y^{\,2}\right)\psi_n=(2n+1)\,\psi_n, \tag{4.7.19}$$

where $x=d\,y$, and $d=\sqrt{\hbar/m\,\omega}$. It is helpful to define the operators

$$a_{\pm}=\frac{1}{\sqrt{2}}\left(\mp\frac{d}{dy}+y\right). \tag{4.7.20}$$

As is easily demonstrated, these operators satisfy the commutation relation

$$[a_+,a_-]=-1. \tag{4.7.21}$$

Using these operators, Equation ([e5.108]) can also be written in the forms

$$a_+\,a_-\,\psi_n=n\,\psi_n, \tag{4.7.22}$$

or

$$a_-\,a_+\,\psi_n=(n+1)\,\psi_n. \tag{4.7.23}$$

The previous two equations imply that

$$a_+\,\psi_n = \sqrt{n+1}\,\psi_{n+1},$$
$$a_-\,\psi_n = \sqrt{n}\,\psi_{n-1}.$$

We conclude that a_+ and a_- are *raising and lowering operators*, respectively, for the harmonic oscillator: that is, operating on the wavefunction with a_+ causes the quantum number n to increase by unity, and vice versa. The Hamiltonian for the harmonic oscillator can be written in the form

$$H = \hbar\,\omega\left(a_+\,a_- + \frac{1}{2}\right), \tag{4.7.24}$$

from which the result

$$H\,\psi_n = (n+1/2)\,\hbar\,\omega\,\psi_n = E_n\,\psi_n \tag{4.7.25}$$

is readily deduced. Finally, Equations ([e5.107]), ([e5.113]), and ([e5.114]) yield the useful expression

$$\int_{-\infty}^{\infty}\psi_m\,x\,\psi_n\,dx = \frac{d}{\sqrt{2}}\int_{-\infty}^{\infty}\psi_m\,(a_+ + a_-)\,\psi_n\,dx = \sqrt{\frac{\hbar}{2\,m\,\omega}}\,(\sqrt{m}\,\delta_{m,n+1} + \sqrt{n}\,\delta_{m,n-1})\,.$$

Contributors and Attributions

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