Problem 2.41

Find the allowed energies of the half harmonic oscillator

$$V(x) = \begin{cases} (1/2)m\omega^2 x^2, & x > 0, \\ \infty, & x < 0. \end{cases}$$

(This represents, for example, a spring that can be stretched, but not compressed.) *Hint:* This requires some careful thought, but very little actual calculation.

Solution

Schrödinger's equation governs the time evolution of the wave function $\Psi(x,t)$.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t), \quad -\infty < x < \infty, \ t > 0$$

Split up the PDE over the intervals that V(x,t) is defined on.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + (\infty)\Psi(x,t), \quad x < 0 \qquad i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{2}m\omega^2x^2\Psi(x,t), \quad x > 0$$

Only $\Psi(x,t) = 0$ satisfies the one for x < 0. Because the wave function must be continuous, $\Psi(0,t) = 0$ is a boundary condition for the remaining PDE on x > 0. Let there be a prescribed initial condition at t = 0.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + \frac{1}{2} m\omega^2 x^2 \Psi(x, t), \quad x > 0$$

$$\Psi(0, t) = 0$$

$$\Psi(x, 0) = \Psi_0(x)$$

To solve Schrödinger's equation on the half-line, apply the method of reflection: Consider the corresponding problem over the whole line, using the odd extension of the initial condition. Doing so automatically satisfies the boundary condition at x=0. The solution for Ψ will then be the restriction of $\overline{\Psi}$ to x>0.

$$i\hbar\frac{\partial\overline{\Psi}}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\overline{\Psi}}{\partial x^2} + \frac{1}{2}m\omega^2x^2\overline{\Psi}(x,t), \quad -\infty < x < \infty$$

$$\overline{\Psi}(x,0) = \Psi_{0_{\rm odd}}(x) = \begin{cases} \Psi_0(x) & \text{if } x > 0 \\ -\Psi_0(-x) & \text{if } x < 0 \end{cases}$$

Since the PDE and its associated boundary conditions (Ψ and its derivatives tend to zero as $x \to \pm \infty$) are linear and homogeneous, the method of separation of variables can be applied. Assume a product solution of the form $\overline{\Psi}(x,t) = \psi(x)\phi(t)$ and plug it into the PDE.

$$i\hbar \frac{\partial}{\partial t} [\psi(x)\phi(t)] = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} [\psi(x)\phi(t)] + \frac{1}{2}m\omega^2 x^2 [\psi(x)\phi(t)]$$

Evaluate the derivatives.

$$i\hbar\psi(x)\phi'(t) = -\frac{\hbar^2}{2m}\psi''(x)\phi(t) + \frac{1}{2}m\omega^2 x^2\psi(x)\phi(t)$$

Divide both sides by $\psi(x)\phi(t)$ to separate variables.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + \frac{1}{2}m\omega^2 x^2$$

The only way a function of t can be equal to a function of x is if both are equal to a constant E.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + \frac{1}{2}m\omega^2 x^2 = E$$

As a result of using the method of separation of variables, the Schrödinger equation has reduced to two ODEs, one in x and one in t.

$$i\hbar \frac{\phi'(t)}{\phi(t)} = E$$

$$-\frac{\hbar^2}{2m} \frac{\psi''(x)}{\psi(x)} + \frac{1}{2}m\omega^2 x^2 = E$$

Values of E for which the boundary conditions are satisfied are called the eigenvalues (or eigenenergies in this context), and the nontrivial solutions associated with them are called the eigenfunctions (or eigenstates in this context). This system was solved using the method of operator factorization in Problem 2.10. Its solution is assumed to be known here.

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega; \quad \phi(t) = e^{-iE_nt/\hbar}; \quad \psi_n(x); \quad n = 0, 1, 2, \dots$$

According to the principle of superposition, the general solution for $\overline{\Psi}$ is a linear combination of $\psi(x)\phi(t)$ over all n.

$$\overline{\Psi}(x,t) = \sum_{n=0}^{\infty} B_n \psi_n(x) e^{-iE_n t/\hbar}$$

Now apply the initial condition to determine the coefficients B_n .

$$\overline{\Psi}(x,0) = \sum_{n=0}^{\infty} B_n \psi_n(x) = \Psi_{0_{\text{odd}}}(x)$$

Multiply both sides by $\psi_m(x)$, where m is a non-negative integer.

$$\sum_{n=0}^{\infty} B_n \psi_n(x) \psi_m(x) = \Psi_{0_{\text{odd}}}(x) \psi_m(x)$$

Integrate both sides with respect to x from $-\infty$ to ∞ .

$$\int_{-\infty}^{\infty} \sum_{n=0}^{\infty} B_n \psi_n(x) \psi_m(x) dx = \int_{-\infty}^{\infty} \Psi_{0_{\text{odd}}}(x) \psi_m(x) dx$$

Bring the constants in front.

$$\sum_{n=0}^{\infty} B_n \int_{-\infty}^{\infty} \psi_n(x) \psi_m(x) dx = \int_{-\infty}^{\infty} \Psi_{0_{\text{odd}}}(x) \psi_m(x) dx$$

Because the eigenstates are orthogonal, this integral on the left is zero for all $n \neq m$. The infinite series consequently yields one term, the n = m one.

$$B_n \int_{-\infty}^{\infty} [\psi_n(x)]^2 dx = \int_{-\infty}^{\infty} \Psi_{0_{\text{odd}}}(x) \psi_n(x) dx$$

Since the eigenstates are normalized, this integral on the left is 1.

$$B_n = \int_{-\infty}^{\infty} \Psi_{0_{\text{odd}}}(x) \psi_n(x) \, dx$$

If n is even, then the eigenstate $\psi_n(x)$ is an even function of x, meaning that B_n is zero because the integrand is odd and the integration interval is symmetric. If n is odd, then the eigenstate $\psi_n(x)$ is an odd function, meaning that the integrand is even and

$$B_n = 2 \int_0^\infty \Psi_{0_{\text{odd}}}(x) \psi_n(x) dx = 2 \int_0^\infty \Psi_0(x) \psi_n(x) dx.$$

Write the general solution for $\overline{\Psi}$ over the even and odd integers separately.

$$\overline{\Psi}(x,t) = \underbrace{\sum_{q=0}^{\infty} B_{2q} \psi_{2q}(x) e^{-iE_{2q}t/\hbar}}_{0} + \sum_{q=1}^{\infty} B_{2q-1} \psi_{2q-1}(x) e^{-iE_{2q-1}t/\hbar}$$

The solution to Schrödinger's equation on the whole line is then

$$\overline{\Psi}(x,t) = \sum_{q=1}^{\infty} B_{2q-1} \psi_{2q-1}(x) e^{-iE_{2q-1}t/\hbar}, \quad -\infty < x < \infty.$$

As planned, take the restriction of $\overline{\Psi}$ to x > 0 in order to get Ψ .

$$\Psi(x,t) = \sum_{q=1}^{\infty} B_{2q-1}\psi_{2q-1}(x)e^{-iE_{2q-1}t/\hbar}, \quad x > 0$$

In conclusion, for the half harmonic oscillator,

$$\Psi(x,t) = \begin{cases} 0 & \text{if } x < 0 \\ \sum_{q=1}^{\infty} B_{2q-1} \psi_{2q-1}(x) e^{-iE_{2q-1}t/\hbar} & \text{if } x > 0 \end{cases}$$
$$= \theta(x) \sum_{q=1}^{\infty} B_{2q-1} \psi_{2q-1}(x) e^{-iE_{2q-1}t/\hbar}.$$

Only the odd energies of the harmonic oscillator are allowed.

$$E_{2q-1} = \left(2q - \frac{1}{2}\right)\hbar\omega, \quad q = 1, 2, \dots$$