1 Harmonic Oscillator

1.1 Introduction

There are three ways to solve the harmonic oscillator problem in quantum mechanics:

- as a conventional eigenvalue problem involving the Schrödinger equation;
- by making a finite matrix approximation to the Hamiltonian and diagonalizing;
- by a rather abstract approach using so-called raising and lowering operators.

All three methods start by nondimensionalizing the problem. The Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{1}{2}\kappa x^2 \tag{1}$$

where p is the momentum operator, m is the mass, κ is the spring constant, and x is the position operator. The classical resonant frequency is $\omega_0 = (\kappa/m)^{1/2}$. Setting $\hbar = 1$, $\kappa = 1$, and $m = 1$, the Hamiltonian becomes

$$H = (p^2 + x^2)/2, \tag{2}$$

or in position space,

$$H = \frac{\delta(x - x')}{2}\left[-\frac{\partial^2}{\partial x^2} + x^2\right]. \tag{3}$$

Notice that the dimensional scalings of operators can be recovered from dimensional analysis since combinations of κ, m, and $\hbar$ raised to various powers yield length, momentum, and energy. In particular, length scales as $\hbar^{1/2}/(\kappa m)^{1/4}$, momentum as $\hbar^{1/2}(\kappa m)^{1/4}$, and energy as $\hbar\omega_0$.

For the nth eigenstate of the Hamiltonian ψ_n,

$$H\psi_n = E_n\psi_n, \tag{4}$$

where E_n is the energy of that state. Solving this equation gives us the energy eigenvalues and eigenvectors for the harmonic oscillator.

1.2 Schrödinger Equation

An alternative way to understand the scaling of the harmonic oscillator problem is to note that the wavenumber squared is given by

$$k^2 = \frac{2m(E - kx^2/2)}{\hbar^2}. \tag{5}$$

setting $m, \kappa, \hbar = 1$ thus results in the scaled, time-independent Schrödinger equation

$$\frac{\partial^2 \psi}{\partial x^2} + (2E - x^2)\psi = 0. \tag{6}$$

1.2.1 Shooting Method

An informative numerical method for solving the Schrödinger equation is called the shooting method. In the case of a potential well such as the harmonic oscillator, the solution must satisfy $\psi \to 0$ as $x \to \pm\infty$. This condition is approximated in the shooting method by requiring $\psi = 0$ for $|x| \gg x_{turn}$, where x_{turn} is the classical turning point for the particle in the potential well:

$$x_{turn} = (2E)^{1/2}. \tag{7}$$

The behavior of the solution in the classically forbidden regions is exponential-like, since $\kappa^2 < 0$ there. In the allowed region, $\kappa^2 > 0$, and the solution is oscillatory.

The Schrödinger equation is second order, and can be broken down into two first order equations by introducing an auxiliary variable, Σ:

$$\frac{\partial \psi}{\partial x} = \Sigma \qquad \frac{\partial \Sigma}{\partial x} = (x^2 - 2E)\psi. \tag{8}$$

These equations are then integrated across the potential. The integrations are started with $\psi = 0$ and $\Sigma = 1$ on the left side and repeated with different values of the energy, E, until a solution with $\psi = 0$ on the right side of the domain is found. The resulting final value of E is an allowed energy for the particle in the potential well. In general there are many values of E that satisfy the right side boundary condition. The RLaB demonstration program **shoot_demo.r** can be used to find the energies of harmonic oscillator states.

Number	Wavefunction	Energy
1	$\exp(-x^2/2)$	0.5
2	$2x\exp(-x^2/2)$	1.5
3	$(4x^2-2)\exp(-x^2/2)$	2.5
4	$(8x^3-12x)\exp(-x^2/2)$	3.5

Table 1: First four solutions to the scaled harmonic oscillator equation.

1.2.2 Analytical Solutions

It turns out that equation (6) actually has analytic solutions. It is easily verified that the solutions shown in table 1 are valid.

1.3 Finite Matrix Approximation

We make a finite difference approximation to equation (3) in this solution to the harmonic oscillator problem. The state function ψ in x-space representation is approximated at a finite number of points (n) separated by Δx, so that $x_l = (l - n/2)\Delta x$, where $l = 1,\ 2,\ \ldots,\ n$. The second derivative of ψ is then

$$\frac{\partial^2\psi}{\partial x^2} \approx \frac{\psi_{l+1} + \psi_{l-1} - 2\psi_l}{\Delta x^2} \tag{9}$$

so the Hamiltonian is

$$H = \frac{1}{2\Delta x^2}\begin{pmatrix} 2 & -1 & 0 & \cdots \\ -1 & 2 & -1 & \cdots \\ 0 & -1 & 2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} + \frac{1}{2}\begin{pmatrix} x_1^2 & 0 & 0 & \cdots \\ 0 & x_2^2 & 0 & \cdots \\ 0 & 0 & x_3^2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{10}$$

The next step is to diagonalize the finite approximation to the Hamiltonian represented by equation (10). Experience shows that the best combination of range and resolution in x occurs when we set $\Delta x \approx n^{1/2}$. The RLaB symmetric eigenvalue solver "eigs" easily handles cases up to $n = 200$ or greater on a fast personal computer. In this case eigenvalues and eigenfunctions up to about $n^{1/2} \approx 14$ are trustworthy, in that the limitations imposed by the numerical method are not exceeded. The RLaB demonstration program **ho_demo.r** solves the harmonic oscillator equation by this method.

1.4 Raising and Lowering Operators

If the position and momentum operators commuted, we could factor the Hamiltonian as $H = (ip + x)(-ip + x)/2$. However, since $[x, p] = i$, we have to write

$$A^- A^+ = (p^2 + x^2 + ipx - ixp)/2 = H - i[x, p]/2 = H + 1/2 \qquad (11)$$

and

$$A^+ A^- = H - 1/2, \qquad (12)$$

where $A^+ \equiv (-ip + x)/\sqrt{2}$ and $A^- \equiv (ip + x)/\sqrt{2}$.

From equations (4), (11), and (12) we see that

$$A^- A^+ \psi_n = (E_n + 1/2)\psi_n \qquad (13)$$

and

$$A^+ A^- \psi_n = (E_n - 1/2)\psi_n. \qquad (14)$$

Multiplying equation (13) by A^+ and comparing with equation (14),

$$A^+ A^-(A^+\psi_n) = (E_n + 1/2)(A^+\psi_n) = [(E_n + 1) - 1/2](A^+\psi_n), \qquad (15)$$

we see that $A^+\psi_n$ is an eigenvector (possibly unnormalized) of the Hamiltonian with energy $E_n + 1$. Tentatively labeling this state $n + 1$ and taking into account the possibility that it isn't normalized, we write

$$A^+\psi_n = C_n^+ \psi_{n+1} \qquad (16)$$

where C_n^+ is a constant adjusted so that ψ_{n+1} *is* normalized. Similar reasoning yields

$$A^-\psi_n = C_n^- \psi_{n-1}. \qquad (17)$$

Since A^+ and A^- respectively take state n and convert it into state $n + 1$ or state $n - 1$, these operators are called *raising* and *lowering* operators. They give us the key to finding a whole ladder of states and their associated energies once one state is defined. In particular, the energies take on the value E_n, $E_n \pm 1$, $E_n \pm 2$, ...

What are the Cs? Since A^+A^- lowers and then raises the state, we find that $A^+A^-\psi_n = C_{n-1}^+ C_n^- \psi_n$. Similarly, $A^-A^+\psi_n = C_{n+1}^- C_n^+ \psi_n$. From this and equations (13) and (14) we conclude that

$$C_n^+ = (E_n + 1/2)^{1/2} \qquad C_n^- = (E_n - 1/2)^{1/2}. \qquad (18)$$

There has to be a lowest energy state to the harmonic oscillator. Thus, the sequence $E_n,\ E_n - 1,\ E_n - 2,\ \ldots$ must end somewhere. Notice that if $E_1 = 1/2$, then from equations (17) and (18) we find

$$A^- \psi_1 = 0. \tag{19}$$

In other words, there is no state ψ_0. Only with this choice of E_1 does the lowering operation terminate. We conclude that the energies for states $n = 1,\ 2,\ 3,\ \ldots$ are $E_n = 0.5,\ 1.5,\ 2.5\ \ldots.$ Equation (19) also gives us a (formal) way of generating the lowest energy eigenstate. Higher states can be generated (formally) by repeatedly solving equation (16) for ψ_{n+1}.

This is a rather abstract way of developing the solution to the harmonic oscillator problem. However, in position space it is easy to show that

$$A^- \psi_1 = \frac{1}{\sqrt{2}} \left(\frac{\partial}{\partial x} + x \right) \psi_1 = 0, \tag{20}$$

with the resulting (unnormalized) solution $\psi_1(x) = \exp(-x^2/2)$. Similarly, the unnormalized $\psi_2(x)$ can be obtained using the raising operator,

$$\psi_2 \propto A^+ \psi_1 = \frac{1}{\sqrt{2}} \left(-\frac{\partial}{\partial x} + x \right) \psi_1 \propto x \exp(-x^2/2), \tag{21}$$

etc.