Chapter 7
Simple Harmonic Oscillator: One Dimension

In the case of piecewise constant potentials, solving the Schrödinger equation was relatively easy. I obtained solutions in the various spatial regions where the potential was constant and matched the wave functions and their derivatives at places where the potential underwent a point jump discontinuity. In certain cases, additional boundary conditions had to be imposed for $x \sim \infty$ and/or $x \sim -\infty$. For *arbitrary* continuous potentials, the Schrödinger equation must be solved as an entity and, in general, such a solution must be carried out numerically. The numerical methods generally involve the use a discretized form of the Schrödinger equation, in which the kinetic energy operator and the potential are approximated on a finite grid of points. Different approaches can then be used to obtain the eigenergies and eigenfunctions.[1] For certain potentials such as the gravitational-like potential $V(x) = mgx$, the smooth potential well potential, $V(x) = -V_0 \operatorname{sech}^2(x/a)$, and the Morse potential (an anharmonic potential that is used to model intermolecular interactions),

$$V(x) = V_0 \left[1 - 2e^{-(x-x_0)/a}\right]^2, \tag{7.1}$$

it is possible to get solutions in terms of so-called *special functions* of mathematical physics. Special functions refer to quantities such as Bessel, Laguerre, hypergeometric, or Hermite functions that have been studied extensively by mathematicians. In this chapter I study the harmonic oscillator potential. As you will see, an analytic form for the eigenfunctions of the harmonic oscillator can be obtained in terms of *Hermite polynomials*.

[1]See, for example, Mohandas Pillai, Joshua Goglio, and Thad Walker, *Matrix Numerov method for solving Schrödinger's equation*, American Journal of Physics **80**, 1017–1019 (2012), and the references therein. See, also, Paolo Giannozzi, *Lecture notes Numerical Methods in Quantum Mechanics*, at http://www.fisica.uniud.it/~giannozz/Corsi/MQ/mq.html.

P.R. Berman, *Introductory Quantum Mechanics*, UNITEXT for Physics,
https://doi.org/10.1007/978-3-319-68598-4_7

The potential for a simple harmonic oscillator (SHO) associated with a particle having mass m subjected to a restoring force $-\sqrt{m\omega^2}x\mathbf{u}_x$ can be written as

$$V(x) = \frac{1}{2}m\omega^2 x^2. \tag{7.2}$$

Aside from this being the potential characterizing a particle bound by an ideal spring, it is the *approximate* potential for any interaction potential that has a point of stable equilibrium located at $x = 0$, since, in the region about $x = 0$,

$$V(x) \approx V(0) + \frac{1}{2!}\left.\frac{d^2V}{dx^2}\right|_{x=0} x^2. \tag{7.3}$$

Near a point of stable equilibrium $d^2V/dx^2\big|_{x=0}$ can be identified with $m\omega^2$ of the equivalent problem of a particle having mass m moving in a SHO potential. For example, in *optical lattices*, standing wave laser fields are used to trap atoms at the bottom of potential wells that can be approximated as harmonic oscillator potentials. The interaction potential between the nuclei of diatomic molecules can also be approximated by a harmonic oscillator potential, giving rise to *vibrational energy levels*.

7.1 Classical Problem

Most likely, you have already studied the dynamics of a classical, simple harmonic oscillator. The harmonic oscillator potential is amazing in that the motion is periodic with (angular) frequency ω, no matter how you start the oscillator. It returns to its initial position and velocity at all integral multiples of its period, $T = 2\pi/\omega$. The particle spends the least amount of time near $x = 0$ since it is moving fastest there and the most amount of time near the endpoints of its orbit,

$$\pm x_{\max} = \pm\sqrt{\frac{2E}{m\omega^2}}, \tag{7.4}$$

where E is the energy of the oscillator.

The position of the oscillator as a function of time is given by

$$x = x_{\max}\cos(\omega t), \tag{7.5}$$

assuming the particle starts with maximum displacement. The time-averaged probability density $P_{\text{class}}(x)$ to find the particle between x and $x + dx$ is just the fraction of a half period that the particle is located between x and $x + dx$, namely

$$P_{\text{class}}(x)dx = \left|\frac{dt}{\pi/\omega}\right| = \left|\frac{\omega\,(dt/dx)\,dx}{\pi}\right|. \tag{7.6}$$

To find dt/dx, I use the equation for conservation of energy

$$\frac{1}{2}m\left(\frac{dx}{dt}\right)^2 + \frac{1}{2}m\omega^2 x^2 = E \tag{7.7}$$

and solve for

$$\frac{dt}{dx} = \frac{1}{\frac{dx}{dt}} = \frac{1}{\sqrt{\frac{2E}{m} - \omega^2 x^2}} \tag{7.8}$$

to obtain

$$P_{\mathrm{class}}(x) = \frac{1}{\pi\sqrt{x_{\max}^2 - x^2}}, \tag{7.9}$$

provided $|x| \le x_{\max}$. For $|x| > x_{\max}$, $P_{\mathrm{class}}(x) = 0$.

As predicted, the probability density is greatest (actually infinite) at the endpoints of the motion ($x = \pm x_{\max}$), and smallest at the equilibrium position ($x = 0$). The *momentum* probability density is smallest at $x = \pm x_{\max}$ (where $p = 0$) and a maximum at $x = 0$ (where $p = \pm |p_{\max}|$). In fact, owing to the symmetry of the Hamiltonian on exchange of momentum and position when both are expressed in dimensionless variables [see Eq. (7.13) below], the time-averaged momentum probability density $W_{\mathrm{class}}(p)$ has the same form as $P_{\mathrm{class}}(x)$, namely

$$W_{\mathrm{class}}(p) = \frac{1}{\pi\sqrt{p_{\max}^2 - p^2}}, \tag{7.10}$$

provided $|p| \le p_{\max} = \sqrt{2mE}$. For $|p| > p_{\max}$, $W_{\mathrm{class}}(p) = 0$. The minimum possible energy of a classical particle in the well is equal to zero.

7.2 Quantum Problem

The Hamiltonian for the quantum problem is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{7.11}$$

It is useful to introduce dimensionless coordinate and momentum variables defined by

$$\hat{\xi} = \sqrt{\frac{m\omega}{\hbar}}\hat{x}; \tag{7.12a}$$

$$\hat{\eta} = \sqrt{\frac{1}{\hbar m\omega}}\hat{p} = \frac{1}{i}\frac{d}{d\xi}, \tag{7.12b}$$

such that

$$\hat{H} = \frac{1}{2}\hbar\omega\left(\hat{\eta}^2 + \hat{\xi}^2\right), \tag{7.13}$$

which is obviously symmetric between the dimensionless momentum and coordinate variables. The commutator of $\hat{\xi}$ and $\hat{\eta}$ is

$$\left[\hat{\xi}, \hat{\eta}\right] = i. \tag{7.14}$$

If I measure energy in units of $\hbar\omega$, I can define a dimensionless Hamiltonian operator $\hat{H}'$ by

$$\hat{H}' = \frac{\hat{H}}{\hbar\omega} = \frac{1}{2}\left(\hat{\eta}^2 + \hat{\xi}^2\right). \tag{7.15}$$

We already know a great deal about the solutions of the oscillator problem. The energy levels are discrete and there is no energy degeneracy. Since the Hamiltonian commutes with the parity operator, the eigenfunctions must also be eigenfunctions of the parity operator, that is, they must be either even or odd functions of x. Moreover we expect the ground state wave function to be a symmetric bell-shaped curve centered at $x = 0$ (though *not* a sin function), the first excited state wave function to be an antisymmetric function with a node at the origin, the second excited state wave function to be symmetric about the origin with two nodes, etc. Without loss of generality I can label the lowest energy state by $n = 0$, the first excited state by $n = 1$, etc.

A lower bound for the ground state energy can be obtained using the uncertainty principle. Since the eigenstates have definite parity, it is clear that

$$\langle\hat{\eta}\rangle_n = \left\langle\hat{\xi}\right\rangle_n = 0 \tag{7.16}$$

for any dimensionless eigenfunction $\tilde{\psi}_n(\xi)$ of $\hat{H}'$. The notation used is

$$\left\langle\hat{O}\right\rangle_n = \int_{-\infty}^{\infty}\left[\tilde{\psi}_n(\xi)\right]^* \hat{O}\tilde{\psi}_n(\xi)d\xi, \tag{7.17}$$

where $\hat{O}$ is some arbitrary operator. From Eqs. (7.15)–(7.17), I can calculate

$$\left\langle\hat{H}'\right\rangle_0 = \frac{1}{2}\left\langle\hat{\eta}^2 + \hat{\xi}^2\right\rangle_0 = \frac{1}{2}\left(\Delta\eta^2 + \Delta\xi^2\right), \tag{7.18}$$

where $\Delta\xi^2$ is the variance of $\hat{\xi}$ and $\Delta\eta^2$ is the variance of $\hat{\eta}$ in the $n = 0$ state. It follows from Eqs. (5.94) and (7.14) that

$$\Delta\eta^2 \geq \frac{1}{4\Delta\xi^2}, \tag{7.19}$$

implying that

$$\epsilon = \frac{E}{\hbar\omega} \geq \frac{1}{2}\left(\frac{1}{4\Delta\xi^2} + \Delta\xi^2\right). \tag{7.20}$$

The minimum value of the right-hand side of this expression occurs for $\Delta\xi^2 = 1/2$; consequently

$$\epsilon \geq \frac{1}{2}\left(\frac{1}{2} + \frac{1}{2}\right) = \frac{1}{2}; \tag{7.21a}$$

$$E \geq \frac{\hbar\omega}{2}. \tag{7.21b}$$

We will see that $\hbar\omega/2$ is the *exact* ground state energy, since the ground state eigenfunction turns out to be a Gaussian (recall that the *only* minimum uncertainty wave function is a Gaussian).

I can also deduce the eigenenergies (to within a constant) by demanding that $\left|\tilde{\psi}(\xi, t)\right|^2$ is a periodic function of time having period $T = 2\pi/\omega$. Since

$$\left|\tilde{\psi}(\xi, t)\right|^2 = \sum_{n,n'} a_n a_{n'}^* \tilde{\psi}_n(\xi) \left[\tilde{\psi}_{n'}(\xi)\right]^* \exp\left[-i\left(E_n - E_{n'}\right) t/\hbar\right], \tag{7.22}$$

periodicity requires that

$$\left(E_n - E_{n'}\right)(2\pi/\omega)/\hbar = 2\pi q, \tag{7.23}$$

where q is an integer. This implies that

$$E_n = \hbar\omega\,(n + C), \tag{7.24}$$

where n is a positive integer or zero and C is a constant that is greater than or equal to $1/2$ [which follows from Eq. (7.21b)]. Equation (7.23) could also be satisfied if $E_n = \hbar\omega\,(n^m + C)$ for a positive integer m, but it is not hard to argue that m must be equal to one. We have already seen that the infinite square well energy levels vary as n^2. Since the SHO potential is less steep than the infinite well, its energy levels must vary with n less rapidly than n^2; the only integral value of m that will work is $m = 1$.

7.2.1 Eigenfunctions and Eigenenergies

For the oscillator problem the Schrödinger equation in dimensionless variables can be written as

$$\frac{1}{2}\left(-\frac{d^2}{d\xi^2}+\xi^2\right)\tilde{\psi}_n(\xi)=\epsilon_n\tilde{\psi}_n(\xi), \tag{7.25}$$

where

$$\epsilon_n=\frac{E_n}{\hbar\omega}. \tag{7.26}$$

Thus, I must solve

$$\frac{d^2\tilde{\psi}_n(\xi)}{d\xi^2}+\left(2\epsilon_n-\xi^2\right)\tilde{\psi}_n(\xi)=0. \tag{7.27}$$

As I often stress, you can solve a differential equation only if you know the solution. However you can make some progress towards a solution by building in the asymptotic form of the wave functions. We know the solution must go to zero as $|x|\to\infty$. In the case of a square well potential, the bound state eigenfunctions vary as $\exp(-\kappa|x|)$ for large $|x|$. Since the oscillator, potential increases with increasing $|x|$, we would expect a faster fall-off for the eigenfunctions.

For $|\xi|\gg 1$, I approximate Eq. (7.27) as

$$\frac{d^2\tilde{\psi}_n(\xi)}{d\xi^2}-\xi^2\tilde{\psi}_n(\xi)=0 \tag{7.28}$$

and guess a solution, $\tilde{\psi}_n(\xi)=e^{-a\xi^2}$. Then

$$\begin{aligned}\frac{d\tilde{\psi}_n(\xi)}{d\xi}&=-2a\xi e^{-a\xi^2};\\ \frac{d^2\tilde{\psi}_n(\xi)}{d\xi^2}&=4a^2\xi^2e^{-a\xi^2}-2ae^{-a\xi^2}\\ &\approx 4a^2\xi^2e^{-a\xi^2}=4a^2\xi^2\tilde{\psi}_n(\xi).\end{aligned} \tag{7.29}$$

If $a=1/2$, $\tilde{\psi}_n(\xi)=e^{-a\xi^2}$ is an approximate solution of Eq. (7.27) for $|\xi|\gg 1$. I build this dependence into the overall solution by setting

$$\tilde{\psi}_n(\xi)=e^{-\xi^2/2}H_n(\xi), \tag{7.30}$$

where $H_n(\xi)$ is a function to be determined.

I already know that $H_n(\xi)$ must be an even or odd function of ξ since the eigenfunctions are also eigenfunctions of the parity operator. I also know that the lowest energy wave function has no node in the classically allowed region, the second energy level has one node, etc. This implies that $H_n(\xi)$ could be a *polynomial* of order n.

Using Eq. (7.30) and substituting

$$\frac{d^2\tilde{\psi}_n(\xi)}{d\xi^2} = -2H_n'(\xi)\xi e^{-\xi^2/2} - H_n(\xi)e^{-\xi^2/2} + \xi^2 H_n(\xi)e^{-\xi^2/2} + H_n''(\xi)e^{-\xi^2/2} \tag{7.31}$$

into Eq. (7.27), I am led to the following differential equation for $H_n(\xi)$:

$$H_n''(\xi) - 2\xi H_n'(\xi) + (2\epsilon_n - 1)\, H_n(\xi) = 0, \tag{7.32}$$

where the primes indicate differentiation with respect to ξ. This is a well-known (to those who know it well) equation of mathematical physics—Hermite's differential equation. It admits polynomial solutions only if

$$2\epsilon_n = 2n + 1, \tag{7.33}$$

where n is a non-negative integer. The polynomial solutions are the only physically acceptable solutions of Hermite's equation that need concern us.[2] In *Mathematica,* the polynomial solutions of Hermite's equation,

$$H_n''(\xi) - 2\xi H_n'(\xi) + 2nH_n(\xi) = 0, \tag{7.34}$$

are designated as HermiteH[n, ξ]. Note that by limiting the solution to polynomials, I already have determined the eigenenergies, since it follows from Eq. (7.33) that

$$\epsilon_n = n + \frac{1}{2}; \qquad n = 0, 1, 2, \ldots . \tag{7.35}$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right); \qquad n = 0, 1, 2, \ldots . \tag{7.36}$$

The energy levels are equally spaced with spacing $\hbar\omega$, a result I had already predicted based on the periodicity of the solution.

[2] The series solutions given in Eqs. (7.41) and (7.42) lead to divergent wave functions as $\xi \sim \pm\infty$ for non-integer n; however, solutions of Eq. (7.27) *do* exist that are regular as $\xi \sim \infty$ (see problems).

You can guess the first few polynomial solutions of Eq. (7.34) with little effort:

$$H_0(\xi) = 1; \tag{7.37}$$

$$H_1(\xi) = 2\xi; \tag{7.38}$$

$$H_2(\xi) = 4\xi^2 - 2; \tag{7.39}$$

$$H_3(\xi) = 8\xi^3 - 12\xi. \tag{7.40}$$

[The Hermite polynomials $H_n(\xi)$ are defined with the convention that the coefficient of the highest power of ξ is 2^n]. Others can be obtained from recursion relations, a series solution, or the so-called generating function. Hermite polynomials are one of a class of *orthogonal polynomials* that can all be treated by similar methods.

I now list several useful properties of the Hermite polynomials. The series solution for the Hermite polynomials for n even is

$$H_n(\xi) = \frac{(-1)^{n/2}\, n!}{(n/2)!}\left[1 - 2\frac{n}{2!}\xi^2 + 2^2\frac{n(n-2)}{4!}\xi^4 - 2^3\frac{n(n-2)(n-4)}{6!}\xi^6 + \cdots\right] \tag{7.41}$$

and for n odd is

$$H_n(\xi) = \frac{(-1)^{(n-1)/2}\, 2n!}{[(n-1)/2]!}\left[\xi - 2\frac{(n-1)}{3!}\xi^3 + 2^2\frac{(n-1)(n-3)}{5!}\xi^5 - \cdots\right]; \tag{7.42}$$

$H_n(\xi)$ is a polynomial of order n having even parity if n is even and odd parity if n is odd. Some recursion relations are:

$$H_n'(\xi) = 2nH_{n-1}(\xi); \tag{7.43a}$$

$$H_{n+1}(\xi) + 2nH_{n-1}(\xi) = 2\xi H_n(\xi); \tag{7.43b}$$

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - H_n'(\xi). \tag{7.43c}$$

The last of these equations allows you to calculate $H_{n+1}(\xi)$ from $H_n(\xi)$ and $H_n'(\xi)$; in other words, it lets you construct all the Hermite polynomials starting from $H_0(\xi) = 1$. The recursion relations will prove very useful in calculating integrals that are needed in perturbation theory involving oscillators.

The Hermite polynomials are orthogonal (the *wave functions* must be orthogonal since there is no degeneracy) if a weighting factor is used in the integrand, namely

$$\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi)H_m(\xi)d\xi = 2^n n!\sqrt{\pi}\,\delta_{n,m}. \tag{7.44}$$

Moreover there is a *generating function* for the Hermite polynomials: A generating function is an analytic function that can be expressed as a power series of some variable multiplied by the corresponding orthogonal polynomial. For the Hermite polynomials, the generating function is

$$F(\xi, q) = e^{-q^2+2q\xi} = \sum_{n=0}^{\infty} \frac{q^n H_n(\xi)}{n!}. \tag{7.45}$$

To evaluate the $H_n(\xi)$, the exponential is expanded and compared term by term with the series. The generating function can be used to evaluate integrals such as the one appearing in Eq. (7.44).

The normalized eigenfunctions for the SHO are

$$\tilde{\psi}_n(\xi) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\xi^2/2} H_n(\xi); \tag{7.46a}$$

$$\psi_n(x) = \frac{1}{\left(\frac{\hbar}{m\omega}\right)^{1/4} \sqrt{2^n n! \sqrt{\pi}}} e^{-\frac{m\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right). \tag{7.46b}$$

It is often useful to rewrite the recursion relations given in Eqs. (7.43) in terms of the wave function, namely

$$\sqrt{2}\frac{d\tilde{\psi}_n(\xi)}{d\xi} = \sqrt{n}\tilde{\psi}_{n-1}(\xi) - \sqrt{n+1}\tilde{\psi}_{n+1}(\xi); \tag{7.47a}$$

$$\sqrt{2}\xi\tilde{\psi}_n(\xi) = \sqrt{n+1}\tilde{\psi}_{n+1}(\xi) + \sqrt{n}\tilde{\psi}_{n-1}(\xi); \tag{7.47b}$$

$$\sqrt{2(n+1)}\tilde{\psi}_{n+1}(\xi) = \xi\tilde{\psi}_n(\xi) - \frac{d\tilde{\psi}_n(\xi)}{d\xi}. \tag{7.47c}$$

The first few dimensionless eigenfunctions are

$$\tilde{\psi}_0(\xi) = \frac{1}{\pi^{1/4}} e^{-\xi^2/2}; \tag{7.48}$$

$$\tilde{\psi}_1(\xi) = \frac{\sqrt{2}\xi}{\pi^{1/4}} e^{-\xi^2/2}; \tag{7.49}$$

$$\tilde{\psi}_2(\xi) = \frac{\left(2\xi^2 - 1\right)}{\pi^{1/4}\sqrt{2}} e^{-\xi^2/2}; \tag{7.50}$$

$$\tilde{\psi}_3(\xi) = \frac{\left(2\xi^3 - 3\xi\right)}{\pi^{1/4}\sqrt{3}} e^{-\xi^2/2}. \tag{7.51}$$

These are graphed in Fig. 7.1. The ground state eigenfunction is a Gaussian, implying that it represents a minimum uncertainty state. It is obvious from the form of the Hamiltonian that the energy is shared equally between the kinetic ($\eta^2/2$) and potential ($\xi^2/2$) energy. Thus, in an eigenstate,

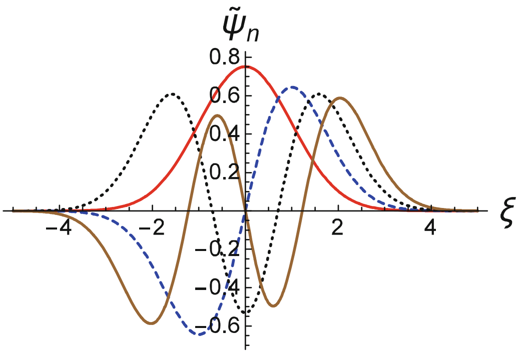

Fig. 7.1 Dimensionless oscillator wave functions, $\tilde{\psi}_n(\xi)$, for $n = 0$ (red, solid), $n = 1$ (blue, dashed), $n = 2$ (black, dotted), and $n = 3$ (brown, solid)

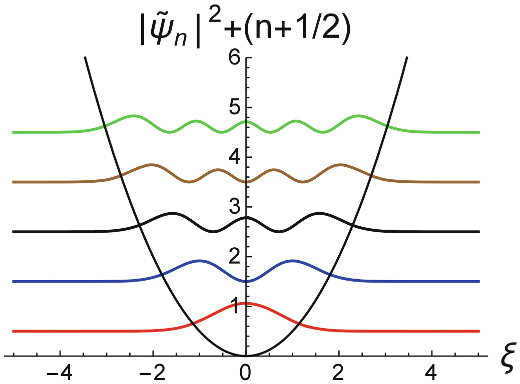

Fig. 7.2 Graphs of $\left[\left|\tilde{\psi}_n(\xi)\right|^2 + (n + 1/2)\right]$ as a function of ξ for $n = 0 - 4$. The harmonic oscillator potential is superposed on the plot

$$\left\langle \hat{\xi}^2 \right\rangle_n = \left\langle \hat{\eta}^2 \right\rangle_n = \left(n + \frac{1}{2}\right). \tag{7.52}$$

In Fig. 7.2, I plot $\left[\left|\tilde{\psi}_n(\xi)\right|^2 + (n + 1/2)\right]$ as a function of ξ for $n = 0 - 4$. Each curve is displaced by the corresponding eigenenergy so that you can see the probability distributions relative to the potential at the appropriate energy. The probability distributions oscillate in the classically allowed region and fall off exponentially in the classically forbidden region.

Finally I look at the eigenfunctions in the large n limit, when we would expect the spatially averaged probability density to approach the classical probability distribution in the classically allowed regime. To make a connection between the classical and quantum problems I set $x = \sqrt{\frac{\hbar}{m\omega}}\xi$, and $E_{\text{class}} = (n + 1/2)\hbar\omega$ in Eq. (7.9) to arrive at the dimensionless probability distribution,

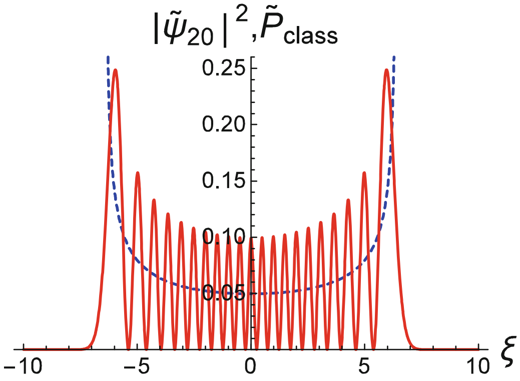

Fig. 7.3 Graphs of the dimensionless classical (blue, dashed) and quantum (red, solid) probability distributions for $n = 20$. The quantum distribution corresponds to the $n = 20$ eigenfunction, while the classical distribution corresponds to an energy $E = 20.5\hbar\omega$

$$\tilde{P}_{\text{class}}(\xi) = \sqrt{\frac{\hbar}{m\omega}} P_{\text{class}}(x) = \frac{1}{\pi\sqrt{2n + 1 - \xi^2}}, \tag{7.53}$$

which is plotted in Fig. 7.3 along with $\left|\tilde{\psi}_n(\xi)\right|^2$ for $n = 20$. You can see that the value of $\left|\tilde{\psi}_{20}(\xi)\right|^2$, averaged over oscillations, is approximately equal to $\tilde{P}_{\text{class}}(\xi)$ in the classically allowed regime.

7.2.2 Time-Dependent Problems

Having solved for the eigenfunctions and eigenvalues, I can construct the time-dependent solution, given some initial condition. The general time-dependent solution is

$$\psi(x, t) = \sum_n b_n e^{-i\left(n+\frac{1}{2}\right)\omega t} \psi_n(x). \tag{7.54}$$

The solution for $|\psi(x, t)|^2$ is periodic with period $T = 2\pi/\omega$, as in the classical problem (the solution for $\psi(x, t)$ is periodic with period $T = 4\pi/\omega$). In contrast to the infinite square well problem, these revivals can be viewed as *classical* in nature since the revival times are integral multiples of the oscillator period, independent of $\hbar$. The dimensionless wave function is

$$\tilde{\psi}(\xi, t) = e^{-i\omega t/2} \sum_{n=0}^{\infty} b_n e^{-in\omega t} \tilde{\psi}_n(\xi), \tag{7.55}$$

with

$$b_n = \int_{-\infty}^{\infty} d\xi \tilde{\psi}_n(\xi)\, \tilde{\psi}(\xi, 0)\,. \tag{7.56}$$

One especially interesting case occurs for an initial wave function

$$\tilde{\psi}(\xi, 0) = \frac{1}{\pi^{1/4}} e^{-(\xi-\xi_0)^2/2}, \tag{7.57}$$

corresponding to the ground state wave function displaced by ξ_0. For this initial wave function,

$$b_n = \frac{1}{\sqrt{2^n n! \pi}} \int_{-\infty}^{\infty} d\xi e^{-\xi^2/2} H_n(\xi) e^{-(\xi-\xi_0)^2/2} = \frac{e^{-\xi_0^2/4}\xi_0^n}{\sqrt{2^n n!}}, \tag{7.58}$$

where the integral could be carried out using the generating function or a table of integrals. Thus, $\tilde{\psi}(\xi, 0)$ can be expanded as

$$\begin{aligned} \tilde{\psi}(\xi, 0) &= e^{-\xi_0^2/4} \sum_{n=0}^{\infty} \frac{\xi_0^n}{\sqrt{2^n n!}} \tilde{\psi}_n(\xi) \\ &= e^{-\left(\xi_0/\sqrt{2}\right)^2/2} \sum_n \frac{\left(\xi_0/\sqrt{2}\right)^n}{\sqrt{n!}} \tilde{\psi}_n(\xi)\,. \end{aligned} \tag{7.59}$$

This wave function is referred to as a *coherent state wave function* and appears in quantum optics, as well. The coherent state wave function has special properties that I will return to when I consider the oscillator using ladder operators and Dirac notation in Chap. 11. From Eqs. (7.55) and (7.58), it follows that

$$\begin{aligned} \tilde{\psi}(\xi, t) &= e^{-i\omega t/2} e^{-\xi_0^2/4} \sum_n \frac{\xi_0^n}{\sqrt{2^n n!}} e^{-in\omega t} \tilde{\psi}_n(\xi) \\ &= e^{-i\omega t/2} \frac{e^{-\xi_0^2/4}}{\pi^{1/4}} e^{-\xi^2/2} \sum_n \frac{1}{n!} \left(\frac{\xi_0}{2} e^{-i\omega t}\right)^n H_n(\xi)\,. \end{aligned} \tag{7.60}$$

The sum is exactly that encountered with the generating function (7.45), so

$$\begin{aligned} \tilde{\psi}(\xi, t) &= e^{-i\omega t/2} \frac{e^{-\xi_0^2/4}}{\pi^{1/4}} e^{-\xi^2/2} \exp\left[2\left(\frac{\xi_0}{2} e^{-i\omega t}\right)\xi - \left(\frac{\xi_0}{2} e^{-i\omega t}\right)^2\right] \\ &= e^{-i\omega t/2} \frac{e^{-\xi_0^2/4}}{\pi^{1/4}} e^{\xi^2/2} \exp\left\{-\left[\xi - \left(\frac{\xi_0}{2} e^{-i\omega t}\right)\right]^2\right\}; \end{aligned} \tag{7.61a}$$

$$\left|\tilde{\psi}(\xi,t)\right|^2 = \frac{e^{-\xi_0^2/2}}{\pi^{1/2}} e^{\xi^2} \exp\left[-2\xi^2 + 2\xi\xi_0\cos(\omega t) - \xi_0^2\cos(2\omega t)/2\right]$$
$$= \frac{1}{\pi^{1/2}} \exp\left[-\xi^2 + 2\xi\xi_0\cos(\omega t) - \frac{\xi_0^2}{2}\left[1+\cos(2\omega t)\right]\right]$$
$$= \frac{1}{\pi^{1/2}} \exp\left[-\xi^2 + 2\xi\xi_0\cos(\omega t) - \xi_0^2\cos^2(\omega t)\right]$$
$$= \frac{1}{\pi^{1/2}} e^{-\left[\xi-\xi_0\cos(\omega t)\right]^2}. \tag{7.61b}$$

The wave packet oscillates in the potential *without changing its envelope*. This is referred to as a *coherent state* since it mimics the behavior of a classical particle. Any spreading of the wave packet resulting from the various momentum components in the packet is exactly compensated by the forces acting on the particle.

7.3 Summary

In obtaining the eigenfunctions and eigenvalues of the SHO, I have solved one of the most important elementary problems in quantum mechanics. Many potentials are modeled as harmonic oscillator potentials, so these solutions are used in a wide range of applications. I did not go through a detailed derivation of the series solution of Hermite's equation, since it can be found in any standard mathematical physics text. Basically one assumes a series solution, obtains the recursion relation for the coefficients, and argues that the series must terminate, or the solution would diverge for large $|x|$. In this way, you obtain the quantization condition.

7.4 Problems

1. How do you know the eigenfunctions of the 1-D oscillator must be even or odd? How many nodes are there for $\tilde{\psi}_n(\xi)$? Based on the general solution of the time-dependent Schrödinger equation and properties of the simple harmonic oscillator, give an argument to show that the frequency difference between any two energy levels must be an integer times ω, where ω is the oscillator frequency. In general, to form a wave packet that corresponds to a particle having energy $E = 1$ J moving in a well having frequency 1 Hz, how many states would be needed?

2. Write the normalized eigenfunctions $\tilde{\psi}_n(\xi)$ of the harmonic oscillator and plot the first four normalized eigenfunctions.

3. For a dimensionless potential $V(\xi)$ varying as

$$V(\xi) = A\,|\xi|^{\mu}\,,$$

where ξ is a dimensionless variable, the (dimensionless) Hamiltonian is

$$\hat{H} = -\frac{1}{2}\frac{d^2}{d\xi^2} + A\,|\xi|^{\mu}\,.$$

For large positive ξ show that the asymptotic form of the wave function is

$$\tilde{\psi}\,(\xi) \sim \exp\left[-a\xi^{\left(\frac{\mu}{2}+1\right)}\right],$$

where a is a constant that depends on μ and A. For $\mu = 0, 2$, show the result agrees with what was obtained for piecewise potentials and the harmonic oscillator, respectively.

4. The *Virial Theorem* in mechanics states that, for closed orbits,

$$\langle T\rangle = \frac{1}{2}\,\langle \mathbf{r}\cdot\nabla V\rangle\,,$$

where T is the kinetic energy. For the 1-D oscillator prove that this implies

$$\langle T\rangle = \langle V\rangle$$

and for the electron in hydrogen $[V(\mathbf{r}) = -K_e/r]$ that

$$\langle T\rangle = -\frac{1}{2}\,\langle V\rangle\,.$$

5. For a 5 mW standing wave laser field having a waist area of $4\,\text{mm}^2$, the potential energy of a ^{85}Rb atom in a "well" of the standing wave field can be approximated as

$$V(x) = 7.9\times 10^{-28}\ \sin^2(kx)\ \text{J},$$

where $k = 2\pi/\lambda$ and $\lambda = 780\,\text{nm}$. Estimate the frequency spacing of the energy levels near the bottom of the well. How cold do the atoms have to be to have most of the atoms in the ground state of the well in thermal equilibrium? Such temperatures can be achieved using techniques of laser cooling.

6. Expand the generating function

$$F(\xi,q) = e^{-q^2+2q\xi} = \sum_{n=0}^{\infty}\frac{q^n H_n(\xi)}{n!}$$

to fourth order in q and show that it gives the correct Hermite polynomials.

7. Given an initial state for the 1-D oscillator

$$\tilde{\psi}(\xi,0) = Ne^{-\xi^2/2}\left(\xi^2+2\right).$$

Find N such that $\tilde{\psi}(\xi,0)$ is normalized. Find $\tilde{\psi}(\xi,t)$. Calculate the average energy in this state.

8. Given a particle having mass m moving in the dimensionless potential (in units of $\hbar\omega$),

$$V(\xi) = \begin{cases} \xi^2/2 & \xi > 0 \\ 0 & \xi < 0 \end{cases},$$

show explicitly that the intensity reflection coefficient is equal to unity. [Hint, for $\xi > 0$, the time-independent Schrödinger equation is

$$\frac{d^2\tilde{\psi}_n(\xi)}{d\xi^2} + \left(2\epsilon_k - \xi^2\right)\tilde{\psi}_n(\xi) = 0,$$

where

$$\epsilon_k = \frac{E_k}{\hbar\omega} = \frac{\hbar k^2}{2m\omega} = \nu_k + \frac{1}{2} > 0.$$

A solution of this equation that goes to zero as $\xi \sim \infty$ is

$$\tilde{\psi}_{\nu_k}(\xi) = D_{\nu_k}\left(\sqrt{2}\xi\right) = 2^{-\nu_k/2}e^{-\xi^2/2}H_{\nu_k}(\xi),$$

where D_ν is a *parabolic cylinder function*. This equation defines Hermite functions H_ν when ν is non-integral. Solve Schrödinger's equation for $\xi < 0$ and $\xi > 0$. Then use the continuity of the wave function and its derivative at $\xi = 0$ to obtain an expression for the reflection coefficient. You may use the fact that $H_\nu(\xi)$ is real and that $dH_\nu/d\xi$ can be calculated using Eq. (7.43a).]