where we have used the fact that $\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 2\hat{a}^\dagger\hat{a} + 1$. Since the expectation values of $\hat{a}^2$ and $\hat{a}^{\dagger 2}$ are zero, $\langle n \mid \hat{a}^2 \mid n\rangle = \langle n \mid \hat{a}^{\dagger 2} \mid n\rangle = 0$, and $\langle n \mid \hat{a}^\dagger\hat{a} \mid n\rangle = n$, we have

$$\langle n \mid \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \mid n\rangle = \langle n \mid 2\hat{a}^\dagger\hat{a} + 1 \mid n\rangle = 2n + 1; \tag{4.186}$$

hence

$$\langle n \mid \hat{X}^2 \mid n\rangle = \frac{\hbar}{2m\omega}\langle n \mid \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \mid n\rangle = \frac{\hbar}{2m\omega}(2n+1), \tag{4.187}$$

$$\langle n \mid \hat{P}^2 \mid n\rangle = \frac{m\hbar\omega}{2}\langle n \mid \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \mid n\rangle = \frac{m\hbar\omega}{2}(2n+1). \tag{4.188}$$

Comparing (4.187) and (4.188) we see that the expectation values of the potential and kinetic energies are equal and are also equal to half the total energy:

$$\boxed{\frac{m\omega^2}{2}\langle n \mid \hat{X}^2 \mid n\rangle = \frac{1}{2m}\langle n \mid \hat{P}^2 \mid n\rangle = \frac{1}{2}\langle n \mid \hat{H} \mid n\rangle.} \tag{4.189}$$

This result is known as the *Virial theorem*.

We can now easily calculate the product $\Delta x\,\Delta p$ from (4.187) and (4.188). Since $\langle\hat{X}\rangle = \langle\hat{P}\rangle = 0$ we have

$$\Delta x = \sqrt{\langle\hat{X}^2\rangle - \langle\hat{X}\rangle^2} = \sqrt{\langle\hat{X}^2\rangle} = \sqrt{\frac{\hbar}{2m\omega}(2n+1)}, \tag{4.190}$$

$$\Delta p = \sqrt{\langle\hat{P}^2\rangle - \langle\hat{P}\rangle^2} = \sqrt{\langle\hat{P}^2\rangle} = \sqrt{\frac{m\hbar\omega}{2}(2n+1)}; \tag{4.191}$$

hence

$$\Delta x\,\Delta p = \left(n + \frac{1}{2}\right)\hbar \quad\Longrightarrow\quad \Delta x\,\Delta p \geq \frac{\hbar}{2}, \tag{4.192}$$

since $n \geq 0$; this is the Heisenberg uncertainty principle.

4.9 Numerical Solution of the Schrödinger Equation

In this section we are going to show how to solve a one-dimensional Schrödinger equation numerically. The numerical solutions provide an idea about the properties of stationary states.

4.9.1 Numerical Procedure

We want to solve the following equation numerically:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \Longrightarrow \frac{d^2\psi}{dx^2} + k^2\psi(x) = 0, \tag{4.193}$$

where $k^2 = 2m[E - V(x)]/\hbar^2$.

First, divide the x-axis into a set of equidistant points with a spacing of $h_0 = \Delta x$, as shown in Figure 4.10a. The wave function $\psi(x)$ can be approximately described by its values at the

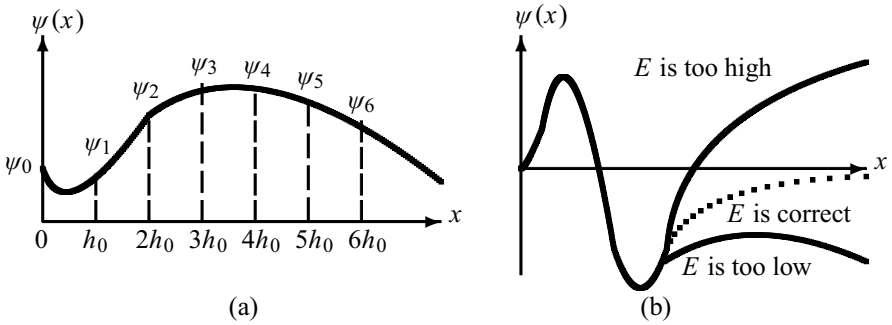

Figure 4.10 (a) Discretization of the wave function. (b) If the energy E used in the computation is too high (too low), the wave function will diverge as $x \to \pm\infty$; but at the appropriate value of E, the wave function converges to the correct values.

points of the grid (i.e., $\psi_0 = \psi(x = 0)$, $\psi_1 = \psi(h_0)$, $\psi_2 = \psi(2h_0)$, $\psi_3 = \psi(3h_0)$, and so on). The first derivative of ψ can then be approximated by

$$\frac{d\psi}{dx} \approx \frac{\psi_{n+1} - \psi_n}{h_0}. \tag{4.194}$$

An analogous approximation for the second derivative is actually a bit tricky. There are several methods to calculate it, but a very efficient procedure is called the *Numerov algorithm* (which is described in standard numerical analysis textbooks). In short, the second derivative is approximated by the so-called three-point difference formula:

$$\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h_0^2} = \psi_n'' + \frac{h_0^2}{12}\psi_n'''' + 0(h_0^4). \tag{4.195}$$

From (4.193) we have

$$\psi_n'''' = \frac{d^2}{dx^2}(-k^2\psi)\bigg|_{x=x_n} = -\frac{(k^2\psi)_{n+1} - 2(k^2\psi)_n + (k^2\psi)_{n-1}}{h_0^2}. \tag{4.196}$$

Using $\psi_n'' = -k_n^2\psi_n$ and substituting (4.196) into (4.195) we can show that

$$\psi_{n+1} = \frac{2\left(1 - \frac{5}{12}h_0^2k_n^2\right)\psi_n - \left(1 + \frac{1}{12}h_0^2k_{n-1}^2\right)\psi_{n-1}}{1 + \frac{1}{12}h_0^2k_{n+1}^2}. \tag{4.197}$$

We can thus assign arbitrary values for ψ_0 and ψ_1; this is equivalent to providing the starting (or initial) values for $\psi(x)$ and $\psi'(x)$. Knowing ψ_0 and ψ_1, we can use (4.197) to calculate ψ_2, then ψ_3, then ψ_4, and so on. The solution of a linear equation, equation (4.197), for either ψ_{n+1} or ψ_{n-1} yields a recursion relation for integrating either *forward* or *backward* in x with a local error $O(h_0^6)$. In this way, the solution depends on two arbitrary constants, ψ_0 and ψ_1, as it should for any second-order differential equation (i.e., there are two linearly independent solutions).

The *boundary conditions* play a crucial role in solving any Schrödinger equation. Every boundary condition gives a linear homogeneous equation satisfied by the wave function or its

derivative. For example, in the case of the infinite square well potential and the harmonic oscillator, the conditions $\psi(x_{min}) = 0$, $\psi(x_{max}) = 0$ are satisfied as follows:

- Infinite square well: $\psi(-a/2) = \psi(a/2) = 0$
- Harmonic oscillator: $\psi(-\infty) = \psi(+\infty) = 0$

4.9.2 Algorithm

To solve the Schrödinger equation with the boundary conditions $\psi(x_{min}) = \psi(x_{max}) = 0$, you may proceed as follows. Suppose you want to find the wave function, $\psi^{(n)}(x)$, and the energy E_n for the nth excited[4] state of a system:

- Take $\psi_0 = 0$ and choose ψ_1 (any small number you like), because the value of ψ_1 must be very close to that of ψ_0.
- Choose a *trial* energy E_n.
- With this value of the energy, E_n, together with ψ_0 and ψ_1, you can calculate iteratively the wave function at different values of x; that is, you can calculate ψ_2, ψ_3, ψ_4, ... How? You need simply to inject $\psi_0 = 0$, ψ_1, and E_n into (4.197) and proceed incrementally to calculate ψ_2; then use ψ_1 and ψ_2 to calculate ψ_3; then use ψ_2 and ψ_3 to calculate ψ_4; and so on till you end up with the value of the wave function at $x_n = nh_0$, $\psi_n = \psi(nh_0)$.
- Next, you need to check whether the ψ_n you obtained is zero or not. If ψ_n is zero, this means that you have made the right choice for the trial energy. This value E_n can then be taken as a possible eigenenergy for the system; at this value of E_n, the wave function converges to the correct value (dotted curve in Figure 4.10b). Of course, it is highly unlikely to have chosen the correct energy from a first trial. In this case you need to proceed as follows. If the value of ψ_n obtained is a nonzero positive number or if it diverges, this means that the trial E_n you started with is larger than the correct eigenvalue (Figure 4.10b); on the other hand, if ψ_n is a negative nonzero number, this means that the E_n you started with is less than the true energy. If the ψ_n you end up with is a positive nonzero number, you need to start all over again with a smaller value of the energy. But if the ψ_n you end up with is negative, you need to start again with a larger value of E. You can continue in this way, improving every time, till you end up with a zero value for ψ_n. Note that in practice there is no way to get ψ_n exactly equal to zero. You may stop the procedure the moment ψ_n is sufficiently small; that is, you stop the iteration at the desired accuracy, say at 10^{-8} of its maximum value.

Example 4.3 (Numerical solution of the Schrödinger equation)
A proton is subject to a harmonic oscillator potential $V(x) = m\omega^2 x^2/2$, $\omega = 5.34 \times 10^{21} s^{-1}$.

(a) Find the exact energies of the five lowest states (express them in MeV).

(b) Solve the Schrödinger equation *numerically* and find the energies of the five lowest states and compare them with the exact results obtained in (a). Note: You may use these quantities: rest mass energy of the proton $mc^2 \simeq 10^3$ MeV, $\hbar c \simeq 200\,\text{MeV fm}$, and $\hbar\omega \simeq 3.5\,\text{MeV}$.

[4] We have denoted here the wave function of the nth excited state by $\psi^{(n)}(x)$ to distinguish it from the value of the wave function at $x_n = nh_0$, $\psi_n = \psi(nh_0)$.

Table 4.1 Exact and numerical energies for the five lowest states of the harmonic oscillator.

n	E_n^{Exact} (MeV)	$E_n^{Numeric}$ (MeV)
0.0	1.750 000	1.749 999 999 795
1.0	5.250 000	5.249 999 998 112
2.0	8.750 000	8.749 999 992 829
3.0	12.250 000	12.249 999 982 320
4.0	15.750 000	15.749 999 967 590

Solution

(a) The exact energies can be calculated at once from $E_n = \hbar\omega(n + \frac{1}{2}) \simeq 3.5(n + \frac{1}{2})$ MeV. The results for the five lowest states are listed in Table 4.1.

(b) To obtain the numerical values, we need simply to make use of the Numerov relation (4.197), where $k_n^2(x) = 2m(E_n - \frac{1}{2}m\omega^2x^2)/\hbar^2$. The numerical values involved here can be calculated as follows:

$$\frac{m^2\omega^2}{\hbar^2} = \frac{(mc^2)^2(\hbar\omega)^2}{(\hbar c)^4} \simeq \frac{(10^3\,\text{MeV})^2(3.5\,\text{MeV})^2}{(200\,\text{MeV fm})^4} = 7.66 \times 10^{-4}\,\text{fm}^{-3}, \quad (4.198)$$

$$\frac{2m}{\hbar^2} = \frac{2mc^2}{(\hbar c)^2} \simeq \frac{2 \times 10^3\,\text{MeV}}{(200\,\text{MeV fm})^2} = 0.05\,\text{MeV}^{-1}\,\text{fm}^{-2}. \quad (4.199)$$

The boundary conditions for the harmonic oscillator imply that the wave function vanishes at $x = \pm\infty$, i.e., at $x_{min} = -\infty$ and $x_{max} = \infty$. How does one deal with infinities within a computer program? For this, we need to choose the numerical values of x_{min} and x_{max} in a way that the wave function would not feel the "edge" effects. That is, we simply need to assign numerical values to x_{min} and x_{max} so that they are far away from the turning points $x_{Left} = -\sqrt{2E_n/(m\omega^2)}$ and $x_{Right} = \sqrt{2E_n/(m\omega^2)}$, respectively. For instance, in the case of the ground state, where $E_0 = 1.75$ MeV, we have $x_{Left} = -3.38$ fm and $x_{Right} = 3.38$ fm; we may then take $x_{min} = -20$ fm and $x_{max} = 20$ fm. The wave function should be practically zero at $x = \pm 20$ fm.

To calculate the energies numerically for the five lowest states, a C++ computer code has been prepared (see Appendix C). The numerical results generated by this code are listed in Table 4.1; they are in excellent agreement with the exact results. Figure 4.11 displays the wave functions obtained from this code for the five lowest states for the proton moving in a harmonic oscillator potential (these plotted wave functions are normalized).

4.10 Solved Problems

Problem 4.1

A particle moving in one dimension is in a stationary state whose wave function

$$\psi(x) = \begin{cases} 0, & x < -a, \\ A(1 + \cos\frac{\pi x}{a}), & -a \le x \le a, \\ 0, & x > a, \end{cases}$$