

the time-dependent Schrödinger equation are given by

$$\Psi(x, t) = \sum_{n=1}^{\infty} \psi_n(x) e^{-iE_n t/\hbar} = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{a}\right) e^{-in^2 E_1 t/\hbar}. \quad (4.83)$$

Zero-point energy

Let us examine why there is no state with zero energy for a square well potential. If the particle has zero energy, it will be at rest inside the well, and this violates Heisenberg's uncertainty principle. By *localizing* or confining the particle to a limited region in space, it will acquire a *finite* momentum leading to a minimum kinetic energy. That is, the localization of the particle's motion to $0 \leq x \leq a$ implies a position uncertainty of order $\Delta x \sim a$ which, according to the uncertainty principle, leads to a minimum momentum uncertainty $\Delta p \sim \hbar/a$ and this in turn leads to a minimum kinetic energy of order $\hbar^2/(2ma^2)$. This is in qualitative agreement with the exact value $E_1 = \pi^2 \hbar^2/(2ma^2)$. In fact, as will be shown in (4.216), an accurate evaluation of Δp_1 leads to a zero-point energy which is equal to E_1 .

Note that, as the momentum uncertainty is inversely proportional to the width of the well, $\Delta p \sim \hbar/a$, if the width decreases (i.e., the particle's position is confined further and further), the uncertainty on \hat{P} will increase. This makes the particle move faster and faster, so the zero-point energy will also increase. Conversely, if the width of the well increases, the zero-point energy decreases, but it will never vanish.

The zero-point energy therefore reflects the necessity of a *minimum motion* of a particle due to localization. The zero-point energy occurs in all bound state potentials. In the case of binding potentials, the lowest energy state has an energy which is higher than the minimum of the potential energy. This is in sharp contrast to classical mechanics, where the lowest possible energy is equal to the minimum value of the potential energy, with zero kinetic energy. In quantum mechanics, however, the lowest state does not minimize the potential alone, but applies to the sum of the kinetic and potential energies, and this leads to a finite ground state or zero-point energy. This concept has far-reaching physical consequences in the realm of the microscopic world. For instance, without the zero-point motion, atoms would not be stable, for the electrons would fall into the nuclei. Also, it is the zero-point energy which prevents helium from freezing at very low temperatures.

The following example shows that the zero-point energy is also present in macroscopic systems, but it is infinitesimally small. In the case of microscopic systems, however, it has a nonnegligible size.

Example 4.1 (Zero-point energy)

To illustrate the idea that the zero-point energy gets larger by going from macroscopic to microscopic systems, calculate the zero-point energy for a particle in an infinite potential well for the following three cases:

- a 100 g ball confined on a 5 m long line,
- an oxygen atom confined to a 2×10^{-10} m lattice, and
- an electron confined to a 10^{-10} m atom.

Solution

- The zero-point energy of a 100 g ball that is confined to a 5 m long line is

$$E = \frac{\hbar^2 \pi^2}{2ma^2} \simeq \frac{10 \times 10^{-68} \text{ J}}{2 \times 0.1 \times 25} \simeq 2 \times 10^{-68} \text{ J} = 1.25 \times 10^{-49} \text{ eV}. \quad (4.84)$$

This energy is too small to be detected, much less measured, by any known experimental technique.

(b) For the zero-point energy of an oxygen atom confined to a 2×10^{-10} m lattice, since the oxygen atom has 16 nucleons, its mass is of the order of $m \simeq 16 \times 1.6 \times 10^{-27}$ kg $\simeq 26 \times 10^{-27}$ kg, so we have

$$E = \frac{10^{-67} \text{ J}}{2 \times 26 \times 10^{-27} \times 4 \times 10^{-20}} \simeq 0.5 \times 10^{-22} \text{ J} \simeq 3 \times 10^{-4} \text{ eV}. \quad (4.85)$$

(c) The zero-point energy of an electron ($m \sim 10^{-30}$ kg) that is confined to an atom ($a \sim 1 \times 10^{-10}$ m) is

$$E = \frac{10^{-67} \text{ J}}{2 \times 10^{-30} \times 10^{-20}} \simeq 5 \times 10^{-18} \text{ J} \simeq 30 \text{ eV}. \quad (4.86)$$

This energy is important at the atomic scale, for the binding energy of a hydrogen electron is about 14 eV. So the zero-point energy is negligible for macroscopic objects, but important for microscopic systems.

4.6.2 The Symmetric Potential Well

What happens if the potential (4.72) is translated to the left by a distance of $a/2$ to become symmetric?

$$V(x) = \begin{cases} +\infty, & x < -a/2, \\ 0, & -a/2 \leq x \leq a/2, \\ +\infty, & x > a/2. \end{cases} \quad (4.87)$$

First, we would expect the energy spectrum (4.76) to remain unaffected by this translation, since the Hamiltonian is invariant under spatial translations; as it contains only a kinetic part, it commutes with the particle's momentum, $[\hat{H}, \hat{P}] = 0$. The energy spectrum is discrete and nondegenerate.

Second, earlier in this chapter we saw that for symmetric potentials, $V(-x) = V(x)$, the wave function of bound states must be either even or odd. The wave function corresponding to the potential (4.87) can be written as follows:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left[\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right] = \begin{cases} \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a}x\right) & (n = 1, 3, 5, 7, \dots), \\ \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) & (n = 2, 4, 6, 8, \dots). \end{cases} \quad (4.88)$$

That is, the wave functions corresponding to odd quantum numbers $n = 1, 3, 5, \dots$ are symmetric, $\psi(-x) = \psi(x)$, and those corresponding to even numbers $n = 2, 4, 6, \dots$ are antisymmetric, $\psi(-x) = -\psi(x)$.

4.7 The Finite Square Well Potential

Consider a particle of mass m moving in the following symmetric potential:

$$V(x) = \begin{cases} V_0, & x < -a/2, \\ 0, & -a/2 \leq x \leq a/2, \\ V_0, & x > a/2. \end{cases} \quad (4.89)$$