1 Particle in a box

We have a particle of mass m confined to a one dimensional region of length a. The state of the particle is given by a wave function $\psi(x,t)$, whose evolution in time is described by the time dependent Schroedinger equation

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x,t). \tag{1}$$

We confine the particle to the box by imposing the boundary conditions

$$\psi(x,t) = 0, x = 0, a \tag{2}$$

1.1 Stationary states

Stationary states play a very important role in quantum mechanics. The probability distribution of a stationary state does not change with time. This means that, if $\psi(x,t)$ is a stationary state, then $|\psi(x,t)|^2$ is time independent.

Suppose $\psi(x,t) = \phi(x)e^{-iEt/\hbar}$. $\phi(x)$ has no time dependence, and $|e^{-iEt/\hbar}|^2 = 1$, so $\psi(x,t)$ is a stationary state. Note that even though the *wave function* ψ itself has time dependence, the *probability distribution* does not.

Plugging $\psi(x,t)$ into the time dependent Schroedinger equation, we get

$$-\frac{\hbar^2}{2m}\partial_x^2\phi(x) = E\phi(x). \tag{3}$$

The solution depends on the boundary conditions. As we saw in class, there is a set of solutions $\{\phi_n\}$ corresponding to discrete energy values $\{E_n\}$; these are given by

$$\begin{aligned} \phi_n(x) &= A_n sin\ k_n x & (4)\\ k_n &= \frac{n\pi}{a} & (5)\\ E_n &= \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}n^2, n = 1, 2, 3, \ldots & (6) \end{aligned}$$

Question: Why do we choose only the positive integers for n? After all, any integer, positive, negative, or zero, leads to a solution of the Schroedinger equation and satisfies the boundary conditions. We throw out the $n = 0$ solution because the wave function would be identically zero: there would be no particle at all! The negative integer question is more subtle; it has to do with the fact that we want only the *linearly independent* stationary states, since the states are specified only up to an overall normalization constant A_n. Clearly $\phi_{-n}(x) = -\phi_n(x)$, so we would not obtain any independent solutions with the negative integers.

1.2 Normalization

Now we want to calculate the normalization constant A_n appearing in the expression for the stationary states. These are fixed by specifying that the integral of the probability density $|\phi(x)|^2$ should equal 1, i.e.

$$\begin{aligned}
\int_0^a dx\ |\phi_n(x)|^2 &= |A_n|^2 \int_0^a dx\ sin^2 \frac{n\pi x}{a} && (7)\\
&= |A_n|^2 \frac{a}{2} && (8)\\
&= 1 && (9)\\
A_n &= \sqrt{\frac{2}{a}}\ e^{i\alpha} && (10)
\end{aligned}$$

In general A_n may be complex; it need only have *norm* 1. But in most cases we can ignore the complex phase factor and make our normalization constants real. So we set $\alpha = 0$ and $A_n = \sqrt{2/a}$.

1.3 Introduction to expectation values

What is the average position, $\bar{x}$? To phrase question more precisely, if 1000 of my friends and I all had a particle in a box, and we measured its position independently, and then took the average of our results, what should the answer be?

In general, when the outcome of an experiment is given by a probability distribution, then the expected (average) value is found by multiplying each possible value by the probability of getting that value, then adding it all up. When there exists only a *discrete* set of possible outcomes, such as when we roll a die, we just add up the finite number of terms to get our answer. When the possible outcomes are *continuous*, such as when we measure the position of a particle, then we multiply each outcome by the *probability density* at that point, and integrate.

Mathematically, if we want to find the average value of some observable $f(x)$ when x is controlled by either a discrete probability distribution p(x) or a probability density $|\phi(x)|^2$, the answer is

$$\overline{f(x)} = \sum_{all\ x} f(x)\ p(x) \tag{11}$$

or

$$\overline{f(x)} = \int dx\ f(x)|\phi(x)|^2 \tag{12}$$

respectively.

For the particle in a box problem, you would put in the probability distribution, pick $f(x) = x$ since position corresponds to the variable x, and integrate from 0 to a, giving the not-too-surprising answer $a/2$.

1.4 Introduction to parity

Parity means what happens to a function when you change the sign of all its variables. Some functions, like $sin(x)$, have *odd* parity, because $sin(-x) = -sin(x)$. On the other hand, $cos(-x) = cos(x)$, so we say $cos(x)$ has *even* parity. Finally, most functions have neither odd nor even parity, such as the function e^x. It is also helpful to notice that the product of two even functions or two odd functions (odd or even under parity) is an even function, while the product of an odd and an even function is odd.

Parit is an example of a symmetry in quantum mechanics, which will be much further developed later on; for now, it can serve as a useful tool for quickly evaluating some expectation values. Notice that when we integrate over *even* bounds, an odd integrand evaluates to 0, while an even integrand gives twice the value over half the range of the integral:

$$\int_{-a}^{a} odd(x) = 0; \tag{13}$$

$$\int_{-a}^{a} even(x) = 2 \int_{0}^{a} even(x) \tag{14}$$

So if you see an odd integrand and even bounds, *or* if you can make a change of variable to put the integral in that form, you can evaluate the result to 0 without doing any more work!

1.5 Orthogonality and completeness

Orthogonality is always defined by means of a *scalar product.* In regular old Cartesian space, two vectors are said to be orthogonal if their dot product $\mathbf{x} \cdot \mathbf{y} = 0$.

In QM, the role of *vectors* is played by square-integrable *functions*. However, we can still define a scalar product. In the case of the square well, the scalar product between wave functions $f(x)$ and $g(x)$ is

$$\int_0^a f(x)^* \, g(x) \, dx \tag{15}$$

The * means complex conjugate. We showed in class that the stationary states of the square well are orthonormal; i.e.

$$\frac{2}{a} \int_0^a sin\left(\frac{n\pi x}{a}\right) \; sin\left(\frac{m\pi x}{a}\right) \; dx = \delta_{nm} \tag{16}$$

The δ_{nm} is the *Kronecker delta*; it equals zero when $n \neq m$ and one when $n = m$.

1.6 General solution of the initial value problem

Once we have found a complete set of stationary states $\phi_n(x)$, and their corresponding energies E_n, then the general solution to the corresponding time-dependent Schroedinger equation can be written as

$$\psi(x,t) \; = \; \sum_n \; c_n(0) \, e^{-iE_n t/\hbar} \, \phi_n(x) \tag{17}$$

where the coefficients $c_n(0)$ are determined by the initial condition:

$$c_n(0) \; = \; \int_{x_1}^{x_2} dx' \, \psi(x',0) \, \phi_n(x') \tag{18}$$