

Tutorial 5 - Measurement and Separation of Variables

Probability

Imagine a room with N people of different ages, so that the number of people of age j is $N(j)$. The total number of people is

$$N = \sum_{j=0}^{\infty} N(j),$$

therefore, the probability to find a person at an age of j is

$$P(j) = \frac{N(j)}{N} = \frac{N(j)}{\sum_j N(j)}.$$

In the case of *continuous variables* there is no sense in specifying the probability for an exact value, but rather a range of values (as small as we'd like), thus

$$P_{ab} = \int_a^b \rho(x) dx,$$

where $\rho(x)$ is the *probability density*. The integral over all space must be 1 - the particle must be somewhere,

$$\int_{-\infty}^{\infty} \rho(x) dx = 1.$$

Measurement in Quantum Mechanics

Considering an observable, represented by an operator \hat{A} , with a set of eigenfunctions $\{\psi_n\}$, such that

$$\hat{A}\psi_n = a_n\psi_n.$$

Since eigenfunction of an observable form a *complete basis*, one may write any wave function as a linear combination of them

$$\psi = \sum_n c_n \psi_n.$$

Thus, the probability for measuring \hat{A} with value a_n is

$$P(A = a_n) = \frac{|c_n|^2}{\sum_n |c_n|^2} = \frac{|\langle \psi_n | \psi \rangle|^2}{\langle \psi | \psi \rangle} = |\langle \psi_n | \psi \rangle|^2,$$

where the last equality assumes that ψ is always normalized.

Once a measurement was made, say $A = a_n$, the system is determined to be in the state ψ_n , so that any successive measurement (immediately after) will result in $A = a_n$.

Note: sometimes two or more states are *degenerate* (share the same eigenvalue), in such case the measurement of an observable collapses the wave function to a combination of the degenerate states.

Question 1:

Consider a “quantum dice”, which is just a quantum description of a regular dice. We define the number operator $\hat{N}\psi_n = n\psi_n$ and the evenness operator $\hat{Z}\psi_n = \frac{1+(-1)^n}{2}\psi_n$.

1. When measuring the number operator, what is the probability of getting $N = 4$?
2. When measuring the evenness operator, what is the probability of getting $Z = 1$?
3. We measure the number operator and get $N = 4$. Afterwards, we measure the evenness operator, what is the value we are going to get?
4. We measure the evenness operator and get $Z = 1$. Afterwards, we measure the number operator. What is the probability of measuring $N = 4$?

Solution:

A dice can be represented by a wave function as follows

$$\psi = \frac{1}{\sqrt{6}}(\psi_1 + \psi_2 + \psi_3 + \psi_4 + \psi_5 + \psi_6),$$

so that $\langle \psi_n, \psi_m \rangle = \delta_{nm}$ and $\langle \psi | \psi \rangle = 1$.

1. The probability of getting $N = 4$ is

$$P(N = 4) = |\langle \psi_4 | \psi \rangle|^2 = \frac{1}{6}.$$

2. The probability of getting $Z = 1$ is the sum of the probabilities

$$P(Z = 1) = P(N = 2) + P(N = 4) + P(N = 6) = |\langle \psi_2 | \psi \rangle|^2 + |\langle \psi_4 | \psi \rangle|^2 + |\langle \psi_6 | \psi \rangle|^2,$$

$$P(Z = 1) = \frac{1}{2}.$$

3. After measuring $N = 4$ the wave function collapses to ψ_4 , thus

$$P_{N=4}(Z = 1) = |\langle \psi_2 | \psi_4 \rangle|^2 + |\langle \psi_4 | \psi_4 \rangle|^2 + |\langle \psi_6 | \psi_4 \rangle|^2 = |\langle \psi_4 | \psi_4 \rangle|^2,$$

$$P_{N=4}(Z = 1) = 1.$$

4. After measuring $Z = 1$ the wave function collapses to the combination of states

$$\psi_{Z=1} = C(\psi_2 + \psi_4 + \psi_6),$$

where C is normalization constant such that $\langle \psi_{Z=1} | \psi_{Z=1} \rangle = 1$, i.e. $C = \frac{1}{\sqrt{3}}$.

Thus,

$$P_{Z=1}(N = 4) = |\langle \psi_4, \psi_{Z=1} \rangle|^2 = \frac{1}{3}.$$

Stationary States

In order to *get* $\Psi(x, t)$ we need to solve the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi,$$

for a specified potential $V(x, t)$. However, for most purposes it is enough to assume a time-independent potential, for which, the Schrödinger equation can be solved by using *separation of variables*, that is

$$\Psi(x, t) = \psi(x) \varphi(t).$$

Note that this is not a general solution, but we will see that we may combine such solutions to form a general one.

Plugging our new solution into the Schrödinger equation reads

$$i\hbar \psi \frac{d\varphi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} \varphi + V\psi\varphi \quad \rightarrow \quad i\hbar \frac{1}{\varphi} \frac{d\varphi}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2\psi}{dx^2} + V.$$

Since the left-hand-side is a function of t alone and the right-hand-side is a function of x alone, the only way for this equation to hold is if both sides are *constant*, which we will denote by E . Therefore we are left with two equations

$$\frac{d\varphi}{dt} = -\frac{iE}{\hbar} \varphi \quad \text{and} \quad \boxed{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V = E\psi}.$$

To conclude: Given a starting wave function $\Psi(x, 0)$, in order to find $\Psi(x, t)$ we take the following steps,

first: solve $\hat{H}\psi = E\psi \quad \rightarrow \quad \{\psi_n\}$ with $\{E_n\}$,

then: fit $\Psi(x, 0) = \sum_n c_n \psi_n(x) \quad \rightarrow \quad \{c_n\}$,

finally: write the solution as $\boxed{\Psi(x, t) = \sum_n c_n \psi_n(x) e^{-i\frac{E_n}{\hbar}t} = \sum_n c_n \Psi_n(x, t)}.$

Additional reading: David Griffiths, Introduction to Quantum Mechanics (3rd edition), Ch. 2.1, p.25-30.

Infinite Square Well

Consider the following potential function

$$V(x) = \begin{cases} 0, & 0 \leq x \leq a, \\ \infty, & \text{else.} \end{cases}$$

Outside the well there is zero probability of finding the particle, $\psi(x) = 0$, whereas inside the well it follows the (time-independent) Schrödinger equation

$$\hat{H}\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad \rightarrow \quad \frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

Here we assume that $E > 0$, otherwise there is no physical solution. This is the *simple harmonic oscillator* equation, for which the general solution is

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

Applying the boundary conditions, we find

$$\psi(0) = 0 \quad \rightarrow \quad A + B = 0,$$

thus

$$\psi(x) = A(e^{ikx} - e^{-ikx}) = A \sin kx,$$

where we absorbed the $(2i)$ factor into A . The second boundary condition yields

$$\psi(a) = 0 \quad \rightarrow \quad A \sin ka = 0,$$

and since $A = 0$ would yield the trivial solution, we are left with

$$k_n = \frac{n\pi}{a}, \quad \text{with } n \in \{1, 2, 3, \dots\}$$

Note that the boundary condition at $\psi(a) = 0$ does not determine the constant A but rather the allowed energies of the system

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2},$$

while the normalization condition is the one to determine A ,

$$\int_0^a \psi \psi^* dx = |A|^2 \int_0^a \sin^2(k_n x) dx = \frac{a|A|^2}{2} = 1 \quad \rightarrow \quad |A| = \sqrt{\frac{2}{a}}.$$

Therefore, inside the well, the solutions are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right).$$

We call the lowest allowed energy the *ground state*, and the others *excited states*. Note that:

- The solutions $\psi_n(x)$ are alternately *even* and *odd*, with respect to the center of the well. (true for *any symmetric* potential function)
- Each successive state has one more *node* (zero-crossing). (true for *all* potential functions)
- The solutions $\psi_n(x)$ are *orthonormal*: (true for *all* potential functions)

$$\int \psi_n^* \psi_m dx = \delta_{mn}.$$

- They set if solutions $\{\psi_n\}$ is *complete*:

$$f(x) = \sum_n c_n \psi_n(x), \quad \text{with} \quad c_n = \int \psi_n^*(x) f(x) dx.$$

The general solution to the infinite square well potential is

$$\Psi(x, t) = \sqrt{\frac{2}{a}} \sum_n c_n \sin\left(\frac{n\pi}{a}x\right) e^{-i\frac{\hbar^2 \pi^2 n^2}{2ma^2}t},$$

and given an initial wave function $\Psi(x, 0)$ we can fit this solution to it by calculating the c_n coefficients

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x, 0) dx.$$

Additional reading: David Griffiths, Introduction to Quantum Mechanics (3rd edition), Ch. 2.2, p.30-37.

Question 2:

Consider a free particle in an infinite well of length L . At time $t = 0$ the particle is prepared in the state

$$\Psi(x, 0) = A \left(\psi_1 + \sqrt{2}\psi_2 + \sqrt{3}\psi_3 + \sqrt{2}\psi_4 + \psi_5 \right).$$

1. Find $|A|$.
2. Find $\Psi(x, t)$.
3. What is the probability of measuring an energy larger than $\frac{2\hbar^2\pi^2}{mL^2}$?
4. What is the probability of measuring a momentum, in absolute value, of $\frac{4\pi\hbar}{L}$?
5. A measurement of the energy of the particle reads $\frac{8\hbar^2\pi^2}{mL^2}$. After this measurement, we measured the particles momentum, in absolute value.
 - (a) What is the probability of having $|p| = \frac{2\pi\hbar}{L}$?
 - (b) What is the probability of having $|p| = \frac{4\pi\hbar}{L}$?

Solution:

1. Using the normalization condition $\langle \Psi | \Psi \rangle = 1$ we have

$$\begin{aligned} \langle \Psi | \Psi \rangle &= |A|^2 \left\langle \left(\psi_1 + \sqrt{2}\psi_2 + \sqrt{3}\psi_3 + \sqrt{2}\psi_4 + \psi_5 \right) \middle| \left(\psi_1 + \sqrt{2}\psi_2 + \sqrt{3}\psi_3 + \sqrt{2}\psi_4 + \psi_5 \right) \right\rangle \\ &= |A|^2 (1 + 2 + 3 + 2 + 1) \\ &= 9|A|^2, \end{aligned}$$

$$\boxed{|A| = \frac{1}{3}}.$$

2. tacking the time dependent exponent factor on each term yields

$$\boxed{\Psi(x, t) = \frac{1}{3} \left(\psi_1 e^{-iE_1 t/\hbar} + \sqrt{2}\psi_2 e^{-iE_2 t/\hbar} + \sqrt{3}\psi_3 e^{-iE_3 t/\hbar} + \sqrt{2}\psi_4 e^{-iE_4 t/\hbar} + \psi_5 e^{-iE_5 t/\hbar} \right), \quad \text{where} \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}}.$$

3. The probability of measuring $H > \frac{2\hbar^2\pi^2}{mL^2}$ is equivalent of measuring $n > 2$, that is

$$\boxed{P \left(H > \frac{2\hbar^2\pi^2}{mL^2} \right) = P(n > 2) = \sum_{n>2} |\langle \psi_n | \Psi \rangle|^2 = \frac{1}{9} (3 + 2 + 1) = \frac{2}{3}}.$$

4. The probability of measuring $p = \frac{4\pi\hbar}{L}$ is equivalent to the probability of measuring $H = p^2/2m = \frac{4^2\pi^2\hbar^2}{2mL^2}$, i.e. $n = 4$, thus

$$\boxed{P \left(p = \frac{4\pi\hbar}{L} \right) = P(n = 4) = |\langle \psi_4 | \Psi \rangle|^2 = \frac{2}{9}}.$$

5. This measurement determines the state of the system to be ψ_4 , therefore

- (a) $P \left(p = \frac{2\pi\hbar}{L} \right) = P(n = 2) = 0$.
- (b) $P \left(p = \frac{4\pi\hbar}{L} \right) = P(n = 4) = 1$.

Question 3:

Consider a Hamiltonian which describes a one dimensional system of two particles of masses m_1 and m_2 , moving in a potential which depends only on the distance between them:

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + V(\hat{x}_1 - \hat{x}_2).$$

Write down Schrödinger equation using the new variables

$$X \equiv \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}, \quad \text{and} \quad x \equiv x_1 - x_2,$$

and interpret the meaning of these variables. Then use separation of variables to find the equations of motion of X and x .

Solution:

Since the time dependent remains the same, we can already use the time-independent Schrödinger equation

$$E\psi = -\frac{\hbar^2}{2m_1} \frac{\partial^2}{\partial x_1^2} \psi - \frac{\hbar^2}{2m_2} \frac{\partial^2}{\partial x_2^2} \psi + V(\hat{x}_1 - \hat{x}_2) \psi.$$

Separation of the two variables means that we assume

$$\psi(x_1, x_2) = \psi(x, X) = \eta(x) \chi(X)$$

In order to rewrite Schrödinger equation in terms of the new parameters we first need to find the transformations:

$$\begin{aligned} \frac{\partial}{\partial x_i} &= \frac{\partial X}{\partial x_i} \frac{\partial}{\partial X} + \frac{\partial x}{\partial x_i} \frac{\partial}{\partial x} = \frac{m_i}{m_1 + m_2} \frac{\partial}{\partial X} \pm \frac{\partial}{\partial x}, \\ \frac{\partial^2}{\partial x_i^2} &= \left(\frac{m_i}{m_1 + m_2} \frac{\partial}{\partial X} \pm \frac{\partial}{\partial x} \right)^2 = \left(\frac{m_i}{m_1 + m_2} \right)^2 \frac{\partial^2}{\partial X^2} \pm 2 \frac{m_i}{m_1 + m_2} \frac{\partial^2}{\partial X \partial x} + \frac{\partial^2}{\partial x^2}, \end{aligned}$$

where the (+) sign corresponds to $i = 1$ and the (-) sign corresponds to $i = 2$. Thus

$$\begin{aligned} E\psi &= -\frac{\hbar^2}{2m_1} \left(\frac{\partial}{\partial x_1} \right)^2 \psi - \frac{\hbar^2}{2m_2} \left(\frac{\partial}{\partial x_2} \right)^2 \psi + V(\hat{x}_1 - \hat{x}_2) \psi \\ &= -\frac{\hbar^2}{2m_1} \left(\left(\frac{m_1}{m_1 + m_2} \right)^2 \frac{\partial^2}{\partial X^2} + \frac{m_1}{m_1 + m_2} \frac{\partial^2}{\partial X \partial x} + \frac{\partial^2}{\partial x^2} \right) \psi \\ &\quad - \frac{\hbar^2}{2m_2} \left(\left(\frac{m_2}{m_1 + m_2} \right)^2 \frac{\partial^2}{\partial X^2} - \frac{m_2}{m_1 + m_2} \frac{\partial^2}{\partial X \partial x} + \frac{\partial^2}{\partial x^2} \right) \psi \\ &\quad + V(x) \psi \\ &= -\frac{\hbar^2}{2(m_1 + m_2)} \frac{\partial^2}{\partial X^2} \psi - \frac{\hbar^2}{2} \left(\frac{m_1 + m_2}{m_1 m_2} \right) \frac{\partial^2}{\partial x^2} \psi + V(x) \psi. \end{aligned}$$

Plugging in our separated function yields

$$E\eta\chi = -\frac{\hbar^2}{2(m_1 + m_2)} \eta\chi'' - \frac{\hbar^2}{2} \left(\frac{m_1 + m_2}{m_1 m_2} \right) \eta''\chi + V(x)\eta\chi,$$

or,

$$E = -\frac{\hbar^2}{2(m_1 + m_2)} \frac{\chi''}{\chi} - \frac{\hbar^2}{2} \left(\frac{m_1 + m_2}{m_1 m_2} \right) \frac{\eta''}{\eta} + V(x).$$

We can identify $M \equiv m_1 + m_2$ as the total mass and $\mu \equiv m_1 m_2 / M$ as the reduced mass, hence the first term corresponds to the kinetic energy of the center of mass E_{cm} , whereas the second term is that of the internal energy of the system. Then we can separate this equation into

$$-\frac{\hbar^2}{2M} \frac{\chi''}{\chi} = E_{\text{cm}} \quad \text{and} \quad -\frac{\hbar^2}{2\mu} \frac{\eta''}{\eta} + V(x) = E - E_{\text{cm}}.$$

Question 4:

Show that for any square integrable wave packet the following relation holds:

$$\int_{-\infty}^{\infty} J(x, t) dx = \frac{\langle \hat{p} \rangle (t)}{m},$$

where $J(x, t)$ is the probability current density, and $\langle \hat{p} \rangle$ is the mean momentum of the particle.

Solution:

Recalling that

$$J(x, t) = \frac{i\hbar}{2m} \left(\Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x} \right), \quad \text{and} \quad \langle \hat{p} \rangle (t) = \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi dx,$$

we have

$$\begin{aligned} \int_{-\infty}^{\infty} J(x, t) dx &= \int_{-\infty}^{\infty} \frac{i\hbar}{2m} \left(\underbrace{\Psi \frac{\partial \Psi^*}{\partial x}}_{\text{IBP}} - \Psi^* \frac{\partial \Psi}{\partial x} \right) dx \\ &= \frac{1}{m} \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi dx, \end{aligned}$$

where the boundary term vanishes as Ψ must be normalizable. Thus

$$\boxed{\int_{-\infty}^{\infty} J(x, t) dx = \frac{\langle \hat{p} \rangle (t)}{m}}.$$