Tutorial 6 - 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

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

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

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

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

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

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

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

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

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

$$\boxed{P_{N=4}\left(Z = 1\right) = 1}.$$

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

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

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

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

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, or 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 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 eave function $\Psi(x,0)$, in order to find $\Psi(x,t)$ we take the following steps,

$$\begin{aligned}&\text{first:}\quad\text{solve } \hat{H}\psi=E\psi\quad\rightarrow\quad\{\psi_n\}\text{ with }\{E_n\}\,,\\&\text{then:}\quad\text{fit } \Psi(x,0)=\sum_n c_n\psi_n(x)\quad\rightarrow\quad\{c_n\}\,,\\&\text{finally:}\quad\text{write the solution as }\boxed{\Psi(x,t)=\sum_n c_n\psi_n(x)\,e^{-i\frac{E_n}{\hbar}t}=\sum_n c_n\Psi_n(x,t)}.\end{aligned}$$

Additional reading: David Griffiths, Introduction to Quantum Mechanics (3^{nd} 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

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

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

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

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

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

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

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

while the normalization condition is the one to determine A,

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

Therefore, inside the well, the solutions are

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

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)

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

- The set of 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

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

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 (3^{nd} 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 then $\frac{2\hbar^2\pi^2}{mL^2}$?
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

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

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

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

$$\boxed{\Psi(x,t) = \frac{1}{3}\left(\psi_1 e^{-iE_1t/\hbar} + \sqrt{2}\psi_2 e^{-iE_2t/\hbar} + \sqrt{3}\psi_3 e^{-iE_3t/\hbar} + \sqrt{2}\psi_4 e^{-iE_4t/\hbar} + \psi_5 e^{-iE_5t/\hbar}\right), \quad \text{where} \quad E_n = \frac{\hbar^2\pi^2n^2}{2ma^2}}.$$

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:

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

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

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

Separation of the two variables means that we assume

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

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

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

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

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

Plugging in our separated function yields

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

or,

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

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

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

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

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

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

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