Introduction to the Schrodinger Equation in One Dimension (Difficult stuff but rewarding when done)

Time Evolution

One way of doing quantum calculations is called the **Schrodinger Picture** and involves the Schrodinger equation for determining wavefunction corresponding to energy eigenstates and for specifying the time evolution of physical quantities.

In this picture

(a) states are represented by ket vectors that depend on time, $|\psi(t)\rangle$
(b) operators $\hat{Q}$ representing observables or measurable quantities are independent of time

We then get a time-dependent expectation value of the form

$$\left\langle \hat{Q}(t) \right\rangle = \langle \psi(t) | \hat{Q} | \psi(t) \rangle \tag{01}$$

Let t be a continuous parameter. We consider a family of unitary operators $\hat{U}(t)$, with the properties

$$\begin{aligned} &\hat{U}(0) = \hat{I} \\ &\hat{U}(t_1 + t_2) = \hat{U}(t_1)\hat{U}(t_2) \end{aligned} \tag{5.7}$$

Transformations such as displacements, rotations and Lorentz boosts clearly satisfy these properties and so it make sense to require them in general.

As we will see, this operator is the time development operator whose existence was one of our postulates and whose form we specified earlier.

Now we consider infinitesimal t. We can then write the infinitesimal version of the unitary transformation (using a Taylor series) as

$$\hat{U}(t) = \hat{I} + \left.\frac{d\hat{U}(t)}{dt}\right|_{t=0} t + O(t^2) \tag{03}$$

Since the unitary operator must satisfy the **unitarity** condition

$$\hat{U}\hat{U}^+ = \hat{I} \qquad \text{for all } t$$

we have

$$\begin{aligned} \hat{U}\hat{U}^+ = \hat{I} &= \left(\hat{I} + \left.\frac{d\hat{U}(t)}{dt}\right|_{t=0} t + \dots \right)\left(\hat{I} + \left.\frac{d\hat{U}^+(t)}{dt}\right|_{t=0} t + \dots \right) \\ &= \hat{I} + \left[\frac{d\hat{U}(t)}{dt} + \frac{d\hat{U}^+(t)}{dt} \right]_{t=0} t + \dots \end{aligned}$$

which implies that

$$\left[\frac{d\hat{U}(t)}{dt}+\frac{d\hat{U}^{+}(t)}{dt}\right]\Bigg|_{t=0}=0$$

If we define

$$\left.\frac{d\hat{U}(t)}{dt}\right|_{t=0}=-i\hat{H} \tag{04}$$

then the condition becomes

$$-i\hat{H}=+(i\hat{H})^{+}=-i\hat{H}^{+}$$

or

$$\hat{H}=\hat{H}^{+} \tag{05}$$

which says that $\hat{H}$ is a Hermitian operator. It is called the **generator** of the family of transformations $\hat{U}(t)$ because it determines these operators uniquely.

Now consider the property

$$\hat{U}(t_1+t_2)=\hat{U}(t_1)\hat{U}(t_2) \tag{06}$$

A **partial derivative** is defined by

$$\frac{\partial f(x,y,z)}{\partial x}=\left.\frac{df(x,y,z)}{dx}\right|_{y,z=\text{constants}}$$

For example, if $f(x,y,z)=x^3y+xy^7z+x^2\sin(z)$ then

$$\frac{\partial f}{\partial x}=3x^2y+y^7z+2x\sin(z)$$
$$\frac{\partial f}{\partial y}=x^3+7xy^6z$$
$$\frac{\partial f}{\partial x}=xy^7+x^2\cos(z)$$

Taking the appropriate partial derivative of equation (06) we have

$$\left.\frac{\partial}{\partial t_1}\hat{U}(t_1+t_2)\right|_{t_1=0}=\left.\frac{d}{dt}\hat{U}(t)\right|_{t=t_2}=\left.\left(\frac{d}{dt_1}\hat{U}(t_1)\right)\right|_{t_1=0}\hat{U}(t_2)=-i\hat{H}\hat{U}(t_2)$$

which is the same as the equation for arbitrary t

$$i\frac{d\hat{U}(t)}{dt}=\hat{H}\hat{U}(t) \tag{07}$$

This equation is satisfied by the unique solution

$$\hat{U}(t)=e^{-i\hat{H}t} \tag{08}$$

which gives us an expression for the time development operator in terms of the Hamiltonian. Formally, this result is called **Stone's theorem.** This is the same form as we specified earlier.

The **Schrodinger picture** follows directly from this discussion of the $\hat{U}(t)$ operator.

Suppose we have some physical system that is represented by the state vector $|\psi(0)\rangle$ at time t = 0 and represented by the state vector $|\psi(t)\rangle$ at time t.

We ask this question. How are these state vectors related to each other? We make the following assumptions (our earlier postulates) :

(1) **every vector** $|\psi(0)\rangle$ such that $\langle\psi(0)|\psi(0)\rangle = 1$ represents a **possible state** at time $t = 0$

(2) **every vector** $|\psi(t)\rangle$ such that $\langle\psi(t)|\psi(t)\rangle = 1$ represents a **possible state** at time t

(3) **every Hermitian operator** represents an **observable** or **measurable** quantity

(4) the properties of the physical system determine the state vectors to **within a phase factor** since $|\phi\rangle = e^{i\alpha}|\psi\rangle$ implies that

$$\langle\phi|\phi\rangle = \langle\psi|e^{-i\alpha}e^{i\alpha}|\psi\rangle = \langle\psi|\psi\rangle = 1$$

(5) $|\psi(t)\rangle$ is **determined** by $|\psi(0)\rangle$

Now, if $|\psi(0)\rangle$ and $|\phi(0)\rangle$ represent two possible states at $t = 0$ and $|\psi(t)\rangle$ and $|\phi(t)\rangle$ represent the **corresponding** states at time t, then

$\left|\langle\phi(0)|\psi(0)\rangle\right|^2$ = probability of finding the system in the state represented by $|\phi(0)\rangle$ given that the system is in the state $|\psi(0)\rangle$ at $t = 0$

and

$\left|\langle\phi(t)|\psi(t)\rangle\right|^2$ = probability of finding the system in the state represented by $|\phi(t)\rangle$ given that the system is in the state $|\psi(t)\rangle$ at t

(6) it makes **physical sense** to assume that these two probabilities should be the same

$$\left|\langle\phi(0)|\psi(0)\rangle\right|^2 = \left|\langle\phi(t)|\psi(t)\rangle\right|^2 \tag{09}$$

Wigner's theorem (linear algebra)then says that there exists a unitary, linear operator $\hat{U}(t)$ such that

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle \tag{10}$$

and an expression of the form

$$\left|\langle\alpha|\hat{U}(t)|\beta\rangle\right|^2 \tag{11}$$

gives the probability that the system is in state $|\alpha\rangle$ at time t given that it was in state $|\beta\rangle$ at time $t=0$.

We assume that this expression is a continuous function of t. As we have already showed, we then have $\hat{U}(t)$ satisfying the equation

$$i\frac{d\hat{U}(t)}{dt} = \hat{H}\hat{U}(t)$$

or

$$\hat{U}(t) = e^{-i\hat{H}t}$$

and thus,

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle \tag{12}$$

which implies the following equation of motion for the state vector

$$\begin{aligned} i\frac{d\hat{U}(t)}{dt}|\psi(0)\rangle &= \hat{H}\hat{U}(t)|\psi(0)\rangle \\ i\frac{d}{dt}|\psi(t)\rangle &= \hat{H}|\psi(t)\rangle \end{aligned} \tag{13}$$

which is the **abstract form** of the **famous Schrodinger equation.** We will derive the standard form of this equation shortly.

As we said earlier, the operator $\hat{U}(t) = e^{-i\hat{H}t}$ is called the **time evolution operator .**

Finally, we can write a time-dependent expectation value as

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle \tag{14}$$

$$\left\langle\hat{Q}(t)\right\rangle = \langle\psi(t)|\hat{Q}|\psi(t)\rangle \tag{15}$$

This is the **Schrodinger picture** where **state vectors change with time** and **operators are constant in time.**

We note that the Schrodinger picture is **not the same** as the Schrodinger equation. The Schrodinger equation involves a mathematical object called the **wave function** which is **one particular representation** of the state vector, namely the **position representation,** as we shall see later. Thus, the Schrodinger equation is applicable **only** to Hamiltonians that describe operators dependent on **external degrees** of freedom like position and momentum. The Schrodinger picture, on the other hand, works with **both internal and external degrees** of freedom and can handle a much wider class of physical systems, as will shall see.

The Schrodinger Wave equation in the Coordinate Representation

To form a **representation** of an abstract linear vector space we must carry out these steps:

(1) Choose a complete, orthonormal set of basis vectors $\{|\alpha_k\rangle\}$

(2) Construct the identity operator $\hat{I}$ as a sum over the one-dimensional subspace projection operators $|\alpha_k\rangle\langle\alpha_k|$

$$\hat{I} = \sum_k |\alpha_k\rangle\langle\alpha_k| \quad (16)$$

(3) Write an arbitrary vector $|\psi\rangle$ as a linear combination or superposition of basis vectors using the identity operator

$$|\psi\rangle = \hat{I}|\psi\rangle = (\sum_k |\alpha_k\rangle\langle\alpha_k|)|\psi\rangle = \sum_k \langle\alpha_k|\psi\rangle|\alpha_k\rangle \quad (17)$$

It is clear from equation (17), that knowledge about the behavior(say in time) of the expansion coefficients $\langle\alpha_k|\psi\rangle$ will tell us the behavior of the state vector $|\psi\rangle$ and allow us to make predictions.

Remember also, that the expansion coefficient is the probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\alpha_k\rangle$.

A particular representation that has become very important in the study of many systems using Quantum Mechanics is formed using the eigenstates of the position operator as a basis. It is called the **coordinate or position representation.** We will restrict our attention to one dimension for simplicity.

The eigenstates $\{|x\rangle\}$ of the position operator $\hat{x}$ satisfy

$$\hat{x}|x\rangle = x|x\rangle \quad (18)$$

where the eigenvalues x are continuous variables in the range $[-\infty,\infty]$. They form the **basis of the coordinate representation.**

Expanding our earlier discussions, in this case, the summations become integrals and we have

$$\hat{I} = \int |x\rangle\langle x|dx \quad (19)$$

$$|\psi\rangle = \hat{I}|\psi\rangle = \int (|x\rangle\langle x|)|\psi\rangle dx = \int \langle x|\psi\rangle|x\rangle dx \quad (20)$$

The expansion coefficient in the coordinate representation is given by

$$\psi(x) = \langle x|\psi\rangle \quad (21)$$

Since the inner product is defined for all states $|x\rangle$, this new object is clearly a function of the eigenvalues x. It will be the **probability amplitude** for finding the particle to be at the point x in 1-dimensional space if it is in the (abstract)state vector $|\psi\rangle$. It is called the **wave function.**

The bra vector corresponding to $|\psi\rangle$ is

$$\langle\psi| = \langle\psi|\hat{I} = \int \langle\psi|x\rangle\langle x|dx = \int \langle x|\psi\rangle^* \langle x|dx \tag{22}$$

The normalization condition takes the form

$$\begin{aligned}\langle\psi|\psi\rangle = 1 = \langle\psi|\hat{I}|\psi\rangle &= \int \langle\psi|x\rangle\langle x|\psi\rangle dx \\ &= \int |\langle x|\psi\rangle|^2 dx = \int |\psi(x)|^2 dx \\ &= \int \psi^*(x)\psi(x)dx\end{aligned} \tag{23}$$

The probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\phi\rangle$, where

$$|\phi\rangle = \hat{I}|\phi\rangle = \int (|x\rangle\langle x|)|\phi\rangle dx = \int \langle x|\phi\rangle|x\rangle dx \tag{24}$$

is given by

$$\begin{aligned}\langle\phi|\psi\rangle &= (\int \langle x|\phi\rangle^* \langle x|dx)(\int \langle x'|\psi\rangle|x'\rangle dx') \\ &= \int dx \int dx' \langle x|\phi\rangle^* \langle x'|\psi\rangle\langle x|x'\rangle\end{aligned}$$

We need the normalization condition $\langle\vec{x}|\vec{x}'\rangle$. We have

$$\begin{aligned}|\psi\rangle &= \int \langle x'|\psi\rangle|x'\rangle dx' \\ \langle x|\psi\rangle &= \int \langle x'|\psi\rangle\langle x|x'\rangle dx' \\ \psi(x) &= \int \psi(x')\langle x|x'\rangle dx'\end{aligned} \tag{25}$$

which implies that

$$\langle\vec{x}|\vec{x}'\rangle = \delta(\vec{x}-\vec{x}') \tag{26}$$

where

$$\begin{aligned}&\delta(x-a) = \begin{cases}\text{undefined} \\ 0 \qquad \text{otherwise}\end{cases} \\ &\int_{-\infty}^{\infty} f(x)\delta(x-a)dx = f(a) \qquad \text{for any function } f(x)\end{aligned} \tag{27}$$

This "function" is called the **Dirac delta function.**

Putting this into equation (25) we have

$$\psi(x) = \int \psi(x')\langle x|x'\rangle dx' = \int \psi(x')\delta(x-x')dx'$$

which is the defining integral.

Thus, the delta function normalization follows from the completeness property of the projection operators.

Using this result we get

$$\langle\phi|\psi\rangle = \int dx \int dx' \langle x|\phi\rangle^* \langle x'|\psi\rangle \delta(x-x')$$
$$= \int \langle x|\phi\rangle^* \langle x|\psi\rangle dx = \int \phi^*(x)\psi(x)dx \quad (28)$$

We formally write the $\hat{x}$ operator using the expansion in eigenvalues and projection operators as

$$\hat{x} = \int \mathrm{x}|x\rangle\langle x|dx \quad (29)$$

We will also need the properties of the linear momentum operator. The eigenstates $\{|p\rangle\}$ of the momentum operator $\hat{p}$ satisfy

$$\hat{p}|p\rangle = p|p\rangle \quad (30)$$

where the eigenvalues p are continuous variables in the range $[-\infty,\infty]$. They form the basis of the **momentum representation.**

As before, we have

$$\hat{I} = \frac{1}{2\pi\hbar}\int |p\rangle\langle p|dp \quad (31)$$

$$|\psi\rangle = \hat{I}|\psi\rangle = \frac{1}{2\pi\hbar}\int (|p\rangle\langle p|)|\psi\rangle dp = \frac{1}{2\pi\hbar}\int \langle p|\psi\rangle|p\rangle dp \quad (32)$$

The expansion coefficient in the momentum representation is

$$\Psi(p) = \langle p|\psi\rangle \quad (33)$$

It is the probability amplitude for finding the particle with momentum p if it is in the state $|\psi\rangle$.

The bra vector corresponding to $|\psi\rangle$ is

$$\langle\psi| = \langle\psi|\hat{I} = \frac{1}{2\pi\hbar}\int \langle\psi|p\rangle\langle p|dp = \frac{1}{2\pi\hbar}\int \langle p|\psi\rangle^*\langle p|dp \quad (34)$$

The normalization condition takes the form

$$\langle\psi|\psi\rangle = 1 = \langle\psi|\hat{I}|\psi\rangle = \frac{1}{2\pi\hbar}\int \langle\psi|p\rangle\langle p|\psi\rangle dp = \frac{1}{2\pi\hbar}\int |\langle p|\psi\rangle|^2 dp$$
$$= \frac{1}{2\pi\hbar}\int |\Psi(p)|^2 dp = \frac{1}{2\pi\hbar}\int \Psi^*(p)\Psi(p)dp \quad (35)$$

The probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\phi\rangle$, where

$$|\phi\rangle = \hat{I}|\phi\rangle = \frac{1}{2\pi\hbar}\int (|p\rangle\langle p|)|\phi\rangle dp = \frac{1}{2\pi\hbar}\int \langle p|\phi\rangle|p\rangle dp$$

is given by

$$\langle\phi|\psi\rangle = \left(\frac{1}{2\pi\hbar}\int\langle p|\phi\rangle^*\langle p|dp\right)\left(\frac{1}{2\pi\hbar}\int\langle p'|\psi\rangle|p'\rangle dp'\right)$$
$$= \frac{1}{(2\pi\hbar)^2}\int dp\int dp'\langle p|\phi\rangle^*\langle p'|\psi\rangle\langle p|p'\rangle$$

The normalization condition follows from

$$|\psi\rangle = \frac{1}{2\pi\hbar}\int\langle p'|\psi\rangle|p'\rangle dp'$$
$$\langle p|\psi\rangle = \frac{1}{2\pi\hbar}\int\langle p'|\psi\rangle\langle p|p'\rangle dp'$$
$$\Psi(p) = \frac{1}{2\pi\hbar}\int\psi(p')\langle p|p'\rangle dp'$$

which implies that

$$\frac{1}{2\pi\hbar}\langle p|p'\rangle = \delta(p-p') \tag{36}$$

Using this result we get

$$\langle\phi|\psi\rangle = \frac{1}{2\pi\hbar}\int dp\int dp'\langle p|\phi\rangle^*\langle p'|\psi\rangle\delta(p-p')$$
$$= \frac{1}{2\pi\hbar}\int\langle p|\phi\rangle^*\langle p|\psi\rangle dp = \frac{1}{2\pi\hbar}\int\Phi^*(p)\Psi(p)dp \tag{37}$$

We formally write the $\hat{p}$ operator using the expansion in eigenvalues and projection operators as

$$\hat{p} = \frac{1}{2\pi\hbar}\int p|p\rangle\langle p|dp \tag{38}$$

We will now derive the connections between the two representation.

We now need to determine the quantity $\langle\vec{x}|\vec{p}\rangle$. This is, in fact, the key result. It will enable us to derive the Schrodinger equation. We will find that

$$\langle\vec{x}|\vec{p}\rangle = e^{i\vec{p}\bullet\vec{x}/\hbar} \tag{39}$$

Derivation:

A representation of the Dirac delta function is

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x-x')}dp = \delta(x-x') \tag{40}$$

By representation it is implied that we can show that

$$\int_{-\infty}^{\infty} f(x)\left[\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x-a)}dp\right]dx = f(a) \quad \text{for any function } f(x)$$

which follows from Fourier transform theory.

Now we can rewrite equation (40) in another way

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x-x')}dp = \delta(x-x') = \langle x|x'\rangle = \langle x|\hat{I}|x'\rangle$$

$$= \langle x|\left[\int_{-\infty}^{\infty} |p\rangle\langle p|dp\right]|x'\rangle = \int_{-\infty}^{\infty}\langle x|p\rangle\langle p|x'\rangle dp = \int_{-\infty}^{\infty}\langle x|p\rangle\langle x'|p\rangle^* dp$$

which is clearly satisfied by (39).

It is not a unique choice, however. It is the choice, however, that allows Quantum mechanics to **make predictions that agree with experiment.**

We might even say that this choice is **another postulate.**

Now, we can use these results to determine the expectation values of operators involving the position and momentum operators.

Since we are interested in the coordinate representation we need only determine the following quantities.

The position operator calculations are straightforward

$$\langle x|\hat{x}|\psi\rangle = x\langle x|\psi\rangle \quad \text{and} \quad \langle x|f(\hat{x})|\psi\rangle = f(x)\langle x|\psi\rangle \tag{41}$$

For the momentum operator we write

$$\langle x|\hat{p}|\psi\rangle = \frac{1}{2\pi\hbar}\int dp\langle x|\hat{p}|p\rangle\langle p|\psi\rangle$$
$$= \frac{1}{2\pi\hbar}\int dp\langle x|p|p\rangle\langle p|\psi\rangle = \frac{1}{2\pi\hbar}\int p\,dp\langle x|p\rangle\langle p|\psi\rangle$$

Using equation (39) we have

$$p\langle x|p\rangle = -i\hbar\frac{d}{dx}\langle x|p\rangle = \langle x|\hat{p}|p\rangle \tag{42}$$

and

$$\langle x|\hat{p}|\psi\rangle = \frac{1}{2\pi\hbar}\int dp\langle x|\hat{p}|p\rangle\langle p|\psi\rangle$$
$$= \frac{1}{2\pi\hbar}\int dp\langle x|p|p\rangle\langle p|\psi\rangle = \frac{1}{2\pi\hbar}\int dp\left[-i\hbar\frac{d}{dx}\langle x|p\rangle\right]\langle p|\psi\rangle \tag{43}$$
$$= \frac{-i}{2\pi}\frac{d}{dx}\int dp\langle x|p\rangle\langle p|\psi\rangle = -i\hbar\frac{d}{dx}\langle x|\psi\rangle$$

We can also show that

$$\langle \vec{x}|\hat{p}^2|\psi\rangle = -\left(-i\hbar\frac{d}{dx}\right)^2\langle \vec{x}|\psi\rangle = -\hbar^2\frac{d^2}{dx^2}\langle \vec{x}|\psi\rangle \tag{44}$$

Using these equations, we can now derive the Schrodinger wave equation.

The Schrodinger wave equation in one dimension is the differential equation that corresponds to the eigenvector/eigenvalue equation for the Hamiltonian operator or the energy operator.

The resulting states are the energy eigenstates. We already saw that energy eigenstates are stationary states and thus have simple time dependence. This property will allow us to find the time dependence of amplitudes for very complex systems in a straightforward way.

We have $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$ where E = a number and

$$\hat{H} = \text{energy operator} = \text{(kinetic energy + potential energy) operators}$$
$$= \frac{\hat{p}^2}{2m} + V(\hat{x})$$

We then have

$$\begin{aligned}
&\langle x|\frac{\hat{p}^2}{2m} + V(\hat{x})|\psi_E\rangle = E\langle x|\psi_E\rangle \\
&\langle x|\frac{\hat{p}^2}{2m}|\psi_E\rangle + \langle x|V(\hat{x})|\psi_E\rangle = E\langle x|\psi_E\rangle \\
&-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\langle x|\psi_E\rangle + V(x)\langle x|\psi_E\rangle = E\langle x|\psi_E\rangle \\
&-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + V(x)\psi_E(x) = E\psi_E(x)
\end{aligned} \tag{45}$$

which is the **time-independent Schrodinger wave equation** in one dimension. The quantity $\psi_E(x) = \langle x|\psi_E\rangle$ is the **wave function** or the **energy eigenfunction** in the **position representation** corresponding to energy E.

The quantity $|\psi_E(x)|^2 = |\langle x|\psi_E\rangle|^2$ represents the probability density to find a particle at coordinate x if it is the state represented by the vector $|\psi_E\rangle$.

Now the energy eigenfunctions have a simple time dependence, as we can see from the following.

Since

$$\hat{U}(t)|\psi_E\rangle = e^{-i\frac{\hat{H}}{\hbar}t}|\psi_E\rangle = e^{-i\frac{E}{\hbar}t}|\psi_E\rangle \tag{46}$$

we have

$$\begin{aligned}
&\langle x|\hat{U}(t)|\psi_E\rangle = \psi_E(x,t) = e^{-i\frac{E}{\hbar}t}\langle x|\psi_E\rangle \\
&\psi_E(x,t) = e^{-i\frac{E}{\hbar}t}\psi_E(x,0)
\end{aligned} \tag{47}$$

Therefore,

$$\begin{aligned}
&-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x,t)}{dx^2} + V(x)\psi_E(x,t) = E\psi_E(x,t) \\
&-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x,t)}{dx^2} + V(\vec{x})\psi_E(x,t) = i\hbar\frac{\partial}{\partial t}\psi_E(x,t)
\end{aligned} \tag{48}$$

which is the **time-dependent Schrodinger wave equation.**

Clearly, system change in time. One change is the collapse process, which is discontinuous (and non-unitary). We have also developed (from postulate #4) a deterministic (unitary) time evolution between measurements.

Between measurements states evolve according to the equation

$$\left|\psi(t)\right\rangle = \hat{U}(t)\left|\psi(0)\right\rangle = e^{-i\hat{H}t/\hbar}\left|\psi(0)\right\rangle$$

For energy eigenstates we found that

$$\left|\psi_E(t)\right\rangle \hat{U}(t)\left|\psi_E(0)\right\rangle = e^{-i\frac{\hat{H}}{\hbar}t}\left|\psi_E(0)\right\rangle = e^{-i\frac{E}{\hbar}t}\left|\psi_E(0)\right\rangle$$

that is, they only change by a phase factor.

Let us look at a simple example to illustrate the process.

We consider a particle with the hardness property but now we place it in an external force that makes the system have a higher energy when the particle is in the hard state $|h\rangle$ than when it is in the soft state $|s\rangle$. We define these two energies to be $+E_0$ for $|h\rangle$ and $-E_0$ for $|s\rangle$. These energies are just the corresponding energy eigenvalues for these two states. Therefoe, the energy operator (in the hard-soft basis) is given by

$$\hat{H} = \begin{pmatrix} +E_0 & 0 \\ 0 & -E_0 \end{pmatrix}$$

Thus, we have

Case #1

$$\left|\psi(0)\right\rangle = |h\rangle$$
$$\left|\psi(t)\right\rangle = e^{-i\hat{H}t/\hbar}|h\rangle = e^{-iE_0t/\hbar}|h\rangle$$

and

Case #2

$$\left|\psi(0)\right\rangle = |s\rangle$$
$$\left|\psi(t)\right\rangle = e^{-i\hat{H}t/\hbar}|s\rangle = e^{iE_0t/\hbar}|s\rangle$$

In either case, if we measure the hardness of this particle at time t, it still has the same value as at t=0, that is, for case #1

$$\left|\left\langle h|\psi(t)\right\rangle\right|^2 = \left|\langle h|e^{-iE_0t/\hbar}|h\rangle\right|^2 = \left|\langle h|h\rangle\right|^2 = 1$$
$$\left|\left\langle s|\psi(t)\right\rangle\right|^2 = \left|\langle s|e^{-iE_0t/\hbar}|h\rangle\right|^2 = \left|\langle s|h\rangle\right|^2 = 0$$

or the hardness of the particle does not change in time if it starts out in a state of definite hardness (they are energy eigenstates).

When the initial state is not an energy eigenstate, that is, when it is a superposition of hard and soft states, the it will change with time. The change will be in the **relative phase** between the components.

We illustrate this below:

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|h\rangle + |s\rangle\right) \to |g\rangle$$

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = \frac{1}{\sqrt{2}}e^{-i\hat{H}t/\hbar}\left(|h\rangle + |s\rangle\right) = \frac{1}{\sqrt{2}}\left(e^{-i\hat{H}t/\hbar}|h\rangle + e^{-i\hat{H}t/\hbar}|s\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\left(e^{-iE_0 t/\hbar}|h\rangle + e^{iE_0 t/\hbar}|s\rangle\right)$$

so that the relative phase is $e^{2iE_0 t/\hbar}$. This state is not an eigenstate of hardness or color! What is the probaility of measuring various results?

Initially:

$$\left|\langle h|\psi(0)\rangle\right|^2 = \frac{1}{2} = \left|\langle s|\psi(0)\rangle\right|^2$$

$$\left|\langle g|\psi(0)\rangle\right|^2 = 1 \quad , \quad \left|\langle m|\psi(0)\rangle\right|^2 = 0$$

At time t:

$$\left|\langle h|\psi(t)\rangle\right|^2 = \left|\langle h|\left(\frac{1}{\sqrt{2}}\left(e^{-iE_0 t/\hbar}|h\rangle + e^{iE_0 t/\hbar}|s\rangle\right)\right)\right|^2 = \left|\frac{1}{\sqrt{2}}e^{-iE_0 t/\hbar}\right|^2 = \frac{1}{2}$$

$$\left|\langle s|\psi(t)\rangle\right|^2 = \left|\langle s|\left(\frac{1}{\sqrt{2}}\left(e^{-iE_0 t/\hbar}|h\rangle + e^{iE_0 t/\hbar}|s\rangle\right)\right)\right|^2 = \left|\frac{1}{\sqrt{2}}e^{iE_0 t/\hbar}\right|^2 = \frac{1}{2}$$

$$\left|\langle g|\psi(t)\rangle\right|^2 = \left|\langle g|\left(\frac{1}{\sqrt{2}}\left(e^{-iE_0 t/\hbar}|h\rangle + e^{iE_0 t/\hbar}|s\rangle\right)\right)\right|^2$$

$$= \left|\frac{1}{\sqrt{2}}e^{-iE_0 t/\hbar}\langle g|h\rangle + \frac{1}{\sqrt{2}}e^{iE_0 t/\hbar}\langle g|s\rangle\right|^2 = \left|\frac{1}{2}e^{-iE_0 t/\hbar} + \frac{1}{2}e^{iE_0 t/\hbar}\right|^2 = \cos^2\frac{2E_0 t}{\hbar}$$

$$\left|\langle m|\psi(t)\rangle\right|^2 = \left|\langle m|\left(\frac{1}{\sqrt{2}}\left(e^{-iE_0 t/\hbar}|h\rangle + e^{iE_0 t/\hbar}|s\rangle\right)\right)\right|^2$$

$$= \left|\frac{1}{\sqrt{2}}e^{-iE_0 t/\hbar}\langle m|h\rangle + \frac{1}{\sqrt{2}}e^{iE_0 t/\hbar}\langle m|s\rangle\right|^2 = \left|\frac{1}{2}e^{-iE_0 t/\hbar} - \frac{1}{2}e^{iE_0 t/\hbar}\right|^2 = \sin^2\frac{2E_0 t}{\hbar}$$

So the probability of measuring the hardness of this particle that was originally in the green state remains 1/2 (as it was at t=0). But much more interesting is the fact that the probability for measurements of color oscillates between probability = 1 for green and probability = 1 for magenta.

So the procedure is the following:

(1) find the energy operator for the physical system

(2) Express the initial state as a superposition of energy eigenstates

(3) Insert the simple time dependence of the energy eigenstate to obtain the time dependence of the state of the system

(4) Determine probability for final measurements by taking appropriate inner products.