

QMS

Week 3 Applications in Simple Quantum Systems 1

In weeks 3/4 we shall consider some simple quantum systems you are already familiar with, as a way of illustrating some of the algebraic structures we have discussed in past two weeks. We will also see how the Dirac formalism of bra/ket vectors applies in these models. Before this, we need to introduce a little more formalism.

1-d case

We have operators \hat{x}, \hat{p} satisfying $[\hat{x}, \hat{p}] = i\hbar$

In this case we expect our Hilbert space to contain states which may have discrete & continuous eigenvalues w.r.t some operators.

For example let's define the position ket $|x\rangle$

$$\hat{x} |x\rangle = x |x\rangle \quad \text{with } x \in \mathbb{R}.$$

(2)

Thus $|x\rangle$ is an example of a ket having continuous eigenvalues x of the Hermitian position operator \hat{x} . It is therefore an example of the ket $|U_2\rangle$ we discussed previously, so that

$$\langle x' | x \rangle = \delta(x' - x) ; \int_{-\infty}^{\infty} dx |x\rangle \langle x| = 1$$

As such, $|x\rangle$ spans our Hilbert Space, so that any state $|4\rangle$ can be expressed as:-

$$|4\rangle = \int dx |x\rangle \langle x| 4 \rangle = \int dx \langle x| 4 \rangle |x\rangle$$

The functions $\langle x| 4 \rangle \equiv 4(x)$ will turn out to be the wave-function of the state $|4\rangle$!

In the basis defined by $|x\rangle$, the momentum operator $\hat{p} \equiv -i\hbar \frac{d}{dx}$, so that

$$\begin{aligned} \hat{p}|4\rangle &= \int dx |x\rangle \langle x| \hat{p}|4\rangle \\ &= \int dx |x\rangle \left(-i\hbar \frac{d}{dx} \langle x| 4 \rangle \right) \end{aligned}$$

(3)

$$\text{so that } \hat{p}|4\rangle \Rightarrow -i\hbar \frac{d\psi(x)}{dx}$$

on the wave-function $\psi|4\rangle$. It's obvious
 that $\hat{x}|4\rangle = x\psi(x)$ - so just multiply
 $\psi(x)$ by x .

Momentum basis

A different but perfectly acceptable basis for
 our Hilbert space is given by the momentum kets
 $|p\rangle$ defined so that

$$\hat{p}|p\rangle = p|p\rangle, \quad p \in \mathbb{R}.$$

It's natural to also define $\langle p'p \rangle = \delta(p-p')$

and $\int_{-\infty}^{\infty} dp |p\rangle \langle p| = 1$.

Again, we may expand any $|4\rangle$ in terms of
 basis $\{|p\rangle\}$:-

$$|4\rangle = \int_{-\infty}^{\infty} dp \langle p|4\rangle |p\rangle$$

(4)

where quite naturally we interpret
 the functions $\langle p | \psi \rangle \equiv \Psi(p)$ - the wave function
 in momentum space.

It is easy to check that $\hat{p} |\psi\rangle \leftrightarrow p \Psi(p)$
 $\hat{x} |\psi\rangle \leftrightarrow i\hbar \frac{d}{dp} \Psi(p)$

Since $\hat{x} = i\hbar \frac{d}{dp}$ in this basis.

Connection between $\{|x\rangle\}$ and $\{|p\rangle\}$ basis

It is quite natural to expect that there should exist some transformation on our Hilbert Space that takes one between the two bases $\{|x\rangle\}$, $\{|p\rangle\}$.

In fact, using the completeness relations for $|x\rangle$ or $|p\rangle$

$$|x\rangle = \int_{-\infty}^{\infty} dp |p\rangle \langle p|x\rangle \quad \text{and} \quad |p\rangle = \int_{-\infty}^{\infty} dx |x\rangle \langle x|p\rangle$$

which means that the functions $\langle p|x\rangle$ occur as expansion coefficients when we express $|x\rangle$ in terms of $|p\rangle$ and $\langle x|p\rangle$ the coefficients when we express $|p\rangle$ in terms of $|x\rangle$.

(5)

$$\text{where } \langle p | c \rangle = (\langle c | p \rangle)^+.$$

What are the functions $\langle c | p \rangle$?

$$\text{well consider } \hat{p} | p \rangle = \int dx | c \rangle \left(-i\hbar \frac{d}{dx} \langle x | p \rangle \right)$$

$$\text{but obviously } \hat{p} | p \rangle = p | p \rangle = \int dx | c \rangle p \langle x | p \rangle$$

$$\Rightarrow -i\hbar \frac{d}{dx} \langle x | p \rangle = p \langle x | p \rangle.$$

$$\text{Solution: } \langle x | p \rangle = N e^{i x p / \hbar} \quad \text{where } N$$

is some overall normalization constant.

What is interesting is that $\langle x | p \rangle$ is the familiar plane-wave solution of the Schrödinger equation - but we havent even introduced this equation yet!

We can easily fix N by following:-

$$\int_{-\infty}^{\infty} \langle x' | p \rangle \langle p | x \rangle dp \xrightarrow{\text{since}} \langle x' | x \rangle \equiv \delta(x' - x)$$

since $\int_{-\infty}^{\infty} dp \langle p | p \rangle = 1$

$$\Rightarrow |N|^2 \int_{-\infty}^{\infty} e^{+ix'p/\hbar} e^{-ixp/\hbar} dp = \delta(x' - x)$$

(6)

The standard representation of $\delta(x'-x)$ in Fourier analysis is

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

$$\Rightarrow N = \boxed{\frac{1}{\sqrt{2\pi\hbar}}} \quad \text{so } \langle x|p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ixp/\hbar}$$

It follows that we now know how to transform between the functions $\psi(x) \leftrightarrow \psi(p)$.

$$\psi(x) = \langle x|\psi \rangle = \int_{-\infty}^{\infty} \langle x|p \rangle \langle p|\psi \rangle dp$$

but $\langle p|\psi \rangle \equiv \psi(p)$

$$\Rightarrow \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp e^{ixp/\hbar} \psi(p)$$

$$\text{Similarly } \psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ixp/\hbar} \psi(x)$$

This is precisely continuous Fourier transformation!

Probability Interpretation

By assumption we let $|\Psi\rangle$ is normalized as $\langle \Psi | \Psi \rangle = 1$. From this it follows that

$$1 = \int_{-\infty}^{\infty} dx \langle \Psi(x) | \Psi(x) \rangle = \int_{-\infty}^{\infty} dx \Psi^*(x) \Psi(x).$$

$\Rightarrow |\langle x | \Psi \rangle|^2 = \langle \Psi | x \rangle \langle x | \Psi \rangle dx$ is the probability that a measurement of position x yields a value in region $x, x+dx$.

Equally, using $\{|p\rangle\}$ basis, $|\langle p | \Psi \rangle|^2 dp$ is the probability that a measurement of momentum yields value in range $p, p+dp$.

Quite generally, if there is any self-adjoint operator \hat{A} acting on our Hilbert space such that its eigenvectors are non-degenerate and form an orthonormal basis

$$\hat{A} |a_i\rangle = a_i |a_i\rangle ; \quad \langle a_i | a_j \rangle = \delta_{ij}$$

(8)

$$\text{Any ket } |\Psi\rangle = \sum_{i=1}^{\infty} \langle a_i | \Psi \rangle |a_i\rangle$$

so that $|\langle a_i | \Psi \rangle|^2$ = probability that a measurement of the observable A yields the value a_i . Technically we needed to make the assumption of non-degenerate eigenstates $|a_i\rangle$, that is, there is only 1 state having eigenvalue a_i , in order to use orthnormality. In the degenerate case, we have to make use of additional operators that commute with \hat{A} (see later).

Time Evolution

So far we have not considered t-dependence - so '| Ψ ' was meant to represent the state of our system at some fixed time $t=t_0$.

Let us use the notation $|\Psi(t_0)\rangle$ to mean this.

An obvious question is how does the state $|\Psi\rangle$ evolve in time?

We introduce an operator $\hat{U}(t-t_0)$ defined so that the state $|\Psi(t)\rangle$ is given in terms of $|\Psi(t_0)\rangle$

$$|\Psi(t)\rangle = \hat{U}(t-t_0) |\Psi(t_0)\rangle$$

Constraints on \hat{U}

$$\text{At } t=t_0 \text{ we have } \langle \Psi(t_0) | \Psi(t_0) \rangle = 1$$

and we require (in order to maintain conservation of probability) that $\langle \Psi(t) | \Psi(t) \rangle = 1, \forall t > t_0$.

$$\begin{aligned} \langle \Psi(t) | \Psi(t) \rangle &= \langle \Psi(t_0) | \hat{U}^\dagger(t-t_0) \hat{U}(t-t_0) | \Psi(t_0) \rangle \\ &= \langle \Psi(t_0) | \Psi(t_0) \rangle. \end{aligned}$$

$$(1) \Rightarrow \hat{U}^\dagger \hat{U} = \hat{I}. \quad \Rightarrow \quad \hat{U} \text{ is a unitary operator}$$

So in quantum mechanics, a state evolves in time through unitary evolution.

The second condition on \hat{U} is that :-

$$(2) \hat{U}(t-t') \hat{U}(t'-t_0) = \hat{U}(t-t_0)$$

$$\int_{t_0}^t = t' + \int_{t'}^t$$

which is basic composition rule.

We can satisfy (1) + (2) if

$$\hat{U}(t-t_0) = e^{i(t-t_0)\hat{H}}$$

where \hat{H} is a hermitian operator $\hat{H}^+ = \hat{H}$

$$\text{check: (1)} \quad \hat{U}^+ \hat{U} = e^{-i(t-t_0)(\hat{H})^+} e^{i(t-t_0)\hat{H}} \\ = e^{-i(t-t_0)\hat{H} + i(t-t_0)\hat{H}} \\ = e^0 = \mathbb{I}.$$

$$(2) \underbrace{e^{i(t-t')\hat{H}}}_{\hat{U}(t-t')} \underbrace{e^{i(t'-t_0)\hat{H}}}_{\hat{U}(t'-t_0)} = e^{i(t-t')\hat{H} + i(t'-t_0)\hat{H}} \\ = \underbrace{e^{i(t-t_0)\hat{H}}}_{\hat{U}(t-t_0)}$$

Note about Exponentiation of Operators

If we consider e^f where f is any function,

then by definition:-

$$e^f = \sum_{n=0}^{\infty} \frac{1}{n!} f^n$$

If instead we have $e^{\hat{A}}$ where \hat{A} is an operator

$$\text{we define } e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{1}{n!} (\hat{A})^n$$

- so the exponentiation of any operator is an operator.

If \hat{A} is a linear operator, then one can easily see so is $e^{\hat{A}}$.

$$e^{\hat{A}} (a|\psi_1\rangle + b|\psi_2\rangle) = a e^{\hat{A}} |\psi_1\rangle + b e^{\hat{A}} |\psi_2\rangle.$$

Some properties:

$$1) [e^{\hat{A}}]^+ = e^{\hat{A}^+}.$$

proof: $\left[\sum_{n=0}^{\infty} (\hat{A})^n / n! \right]^+ = \sum_{n=0}^{\infty} [(\hat{A})^n]^+ / n! = e^{\hat{A}^+}$

but $[(\hat{A})^n]^+ = (\hat{A}^+)^n$ (just use $(\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+$ repeatedly)

2) If \hat{A} and \hat{B} are any two operators such that $[\hat{A}, \hat{B}] = 0$ then

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B}}$$

sketch proof: $\left(\sum_{n=0}^{\infty} (\hat{A})^n / n! \right) \left(\sum_{m=0}^{\infty} (\hat{B})^m / m! \right) = \sum_{n,m=0}^{\infty} (\hat{A})^n (\hat{B})^m / n! m!$

Binomial expansion $(\hat{A} + \hat{B})^n = \sum_{k=0}^n (\hat{A})^k (\hat{B})^{n-k} \binom{n}{k}$

where $\binom{n}{k} = \frac{n!}{k!(n-k)!}$ → use to show rhs

$$= \sum_{p=0}^{\infty} (\hat{A} + \hat{B})^p / p!$$

$$= e^{\hat{A} + \hat{B}}$$

N.B.

If $[\hat{A}, \hat{B}] \neq 0$ then $e^{\hat{A}} e^{\hat{B}} \neq e^{\hat{A} + \hat{B}}$

- indeed $e^{\hat{A}} e^{\hat{B}} \neq e^{\hat{B}} e^{\hat{A}}$.

$$3) \quad \frac{d}{dt} e^{t\hat{A}} = \hat{A} e^{t\hat{A}} \quad [\text{proof-exercise}]$$

$$4) \quad \text{If } [\hat{A}, \hat{B}] = 0 \quad \text{then } [\hat{B}, e^{\hat{A}}] = 0$$

indeed $[\hat{B}, f(\hat{A})] = 0$ where $f(\hat{A})$ is
a function that has a power series expanded.

Returning to evolution operator $U(t-t_0)$ -

question remains what is $\hat{\Omega}$?

Answer: $\boxed{\hat{\Omega} = -\hat{H}/\hbar}$, \hat{H} the Hamiltonian operator.

Reason one can see in different ways. E.g.

in classical physics Hamilton's equations of motion
indicates $H(x, p)$ is responsible for t-evolution

$$\text{via the equations } \dot{x} = -\{H, x\}_{PB}, \quad \dot{p} = -\{H, p\}_{PB}. \quad (14)$$

where $\{, \}_{PB}$ is the Poisson bracket.

$$\hat{J}^2 = -\hat{H}/\hbar; \quad \boxed{\hat{U}(t-t_0) = e^{-i(t-t_0)/\hbar} \hat{H}}$$

the factor of \hbar is needed to make the exponent a dimensionless quantity.

So the ket $|4(t)\rangle$ representing the state of the system at time t is:-

$$|4(t)\rangle = e^{-i(t-t_0)/\hbar} |4(t_0)\rangle.$$

It follows that $\boxed{\langle x | 4(t) \rangle = \Psi(x, t)}$

corresponds to the t -dependent wave-function.

We can now derive an equation for $\Psi(x, t)$:-

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \langle x | 4(t) \rangle &= i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \langle x | i\hbar \frac{d}{dt} (U(t-t_0)) | 4(t_0) \rangle \\ &= \langle x | \hat{H} | 4(t) \rangle \\ &= \hat{H}(x, p = i\hbar \frac{\partial}{\partial x}) \langle x | 4(t) \rangle \end{aligned}$$

so that $i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H} \Psi(x,t)$.

where in \hat{H} we understand $\hat{p} = -i\hbar \frac{\partial}{\partial x}$.

This is the t -dependent Schrödinger equation!

So the evolution operator $\hat{U}(t-t_0)$ generates automatically a solution of the Schrödinger equation, once we know the state of the system $|\Psi(t_0)\rangle$ at some fixed time t_0 .

Expectation values and Heisenberg — Schrödinger pictures

Let's take $t=t_0$. Given an observable \hat{A} , the expectation value at $t=0$ is:-

$$\langle \Psi(t_0) | \hat{A} | \Psi(t_0) \rangle.$$

Here \hat{A} is assumed not to explicitly depend on time. At a time $t > t_0$ we have

$$\langle \Psi(t) | \hat{A} | \Psi(t) \rangle$$

(16)

Now using completeness relation $\int_{-\infty}^{\infty} dx |x\rangle \langle x| = 1$

$$\begin{aligned}\langle \Psi(t_0) | \hat{A} | \Psi(t_0) \rangle &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \langle \Psi(t_0) | x \rangle \langle x | \hat{A} | x' \rangle \langle x' | \Psi(t_0) \rangle \\ &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \Psi^*(x, t_0) \langle x | \hat{A} | x' \rangle \Psi(x', t_0)\end{aligned}$$

$\langle x | \hat{A} | x' \rangle$ 'represents' the operator \hat{A} in the position vector basis.

$$\text{E.g. if } \hat{A} = \hat{x} ; \quad \langle x | \hat{A} | x' \rangle = \langle x | \hat{x} | x' \rangle \\ = x' \langle x | x' \rangle \\ = x' \delta(x-x')$$

$$\Rightarrow \langle \Psi(t_0) | \hat{A} | \Psi(t_0) \rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \Psi^*(x, t_0) x' \delta(x-x') \Psi(x', t_0) \\ = \int_{-\infty}^{\infty} dx \Psi^*(x, t_0) x \Psi(x, t_0)$$

- i.e. just familiar expression from Schrödinger quantum mechanics.

$$\text{Similarly, } \langle \Psi(t) | \hat{x} | \Psi(t) \rangle = \int_{-\infty}^{\infty} dx \Psi^*(x, t) x \Psi(x, t)$$

Clearly this generalizes to any observable $\hat{A}(\hat{x}, \hat{p})$

$$\langle \psi | \hat{A}(\hat{x}, \hat{p}) | \psi' \rangle = \hat{A}(x, \hat{p} = -i\hbar \frac{\partial}{\partial x}) \delta(x-x')$$

$$\Rightarrow \langle \psi(t) | \hat{A} | \psi(t') \rangle = \int_{-\infty}^{\infty} dx \Psi_{(x,t)}^* \hat{A}(x, p = -i\hbar \frac{\partial}{\partial x}) \Psi_{(x,t')}$$

- again, familiar from Schrödinger Q.M.

There is nothing 'special' about $\{|x\rangle\}$ basis. We could have repeated all above but using $\{|p\rangle\}$ basis.

The point is the result $\langle \psi(t) | \hat{A} | \psi(t') \rangle$ should not depend on choice of basis vectors we choose.

The Dirac formulation makes this manifest, because the ket $|\psi(t_0)\rangle$ makes no reference to any particular basis.

To compute $\langle \psi(t) | \hat{A} | \psi(t') \rangle$ all we need to know is:- 1) $|\psi(t_0)\rangle$ - the state of the system at $t=t_0$.
 2) \hat{H} - the Hamiltonian.
 3) The observable \hat{A} .

None of the data 1)-3) makes reference to a particular basis of our Hilbert Space!

Returning to $\langle \Psi(t) | \hat{A} | \Psi(t) \rangle$ we see that

$$\begin{aligned}\langle \Psi(t) | \hat{A} | \Psi(t) \rangle &= \langle \Psi(t_0) | \hat{U}^\dagger(t-t_0) \hat{A} \hat{U}(t-t_0) | \Psi(t_0) \rangle \\ &\equiv \langle \Psi(t_0) | \hat{A}(t-t_0) | \Psi(t_0) \rangle.\end{aligned}$$

where $\hat{A}(t-t_0) = \hat{U}^\dagger(t-t_0) \hat{A} \hat{U}(t-t_0)$

or

$$\boxed{\hat{A}(t) = \hat{U}^\dagger(t) \hat{A}(t=0) \hat{U}(t)}$$

So it's clear we can always think of the system as being in the state $|\Psi(t_0)\rangle$ - but that observable corresponding to operator \hat{A} evolve in time according to the above equation.

Since $\hat{U}(t) = e^{-it/\hbar \hat{H}}$

$$\frac{d\hat{A}(t)}{dt} = -i\hbar [\hat{A}(t), \hat{H}] \quad - \text{Heisenberg equation motion}$$

This gives rise to the 'Heisenberg' picture or formalism in Q.M. By contrast, in the Schrödinger picture, the states $|\psi(t)\rangle$ are imagined to evolve in time, but that operators corresponding to physical observables, \hat{A} are t -independent.

The two pictures are equivalent!

Extension to 3d

It should be obvious that we can extend all the above discussions to 3d in a straightforward way, $\hat{x} \leftrightarrow \vec{x} = (\hat{x}, \hat{y}, \hat{z})$; $\hat{p} \rightarrow \vec{p} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$

$|\vec{x}\rangle$ satisfy $\hat{x}|\vec{x}\rangle = \vec{x}|\vec{x}\rangle$; $\vec{p} = i\hbar \vec{\nabla}$

completeness: $\int d^3x |\vec{x}\rangle \langle \vec{x}| = 1$

$$\langle \vec{x} | \vec{x}' \rangle = \delta^{(3)}(\vec{x} - \vec{x}')$$

$$\Psi(\vec{x}, t_0) = \langle \vec{x} | \psi(t_0) \rangle; \quad \Psi(\vec{x}, t) = \langle \vec{x} | \hat{U}(t-t_0) \psi(t_0) \rangle$$

Similarly $\int d^3p \ |\vec{p}\rangle \langle \vec{p}| = 1$

$$\langle \vec{p} | \vec{p}' \rangle = \delta^{(3)}(\vec{p} - \vec{p}')$$

$$\Psi(\vec{p}, t_0) = \langle \vec{p} | \Psi(t_0) \rangle ; \quad \Psi(\vec{p}, t) = \langle \vec{p} | \hat{U}(t-t_0) | \Psi(t_0) \rangle$$

$$\hat{\vec{p}} |\vec{p}\rangle = \vec{p} |\vec{p}\rangle , \quad \vec{x} = -i\hbar \frac{\partial}{\partial \vec{p}}$$

N.B. $|\vec{x}\rangle$ is not a vector in 3d ! ; Similarly
 $|\vec{p}\rangle$ not a vector in 3d .

(you should think of $|\vec{x}\rangle = |x, y, z\rangle$; similarly
 $|\vec{p}\rangle = |p_x, p_y, p_z\rangle$)
