Postulates of QM, Part IV

Postulate 6:

The time evolution of state $|\psi\rangle$ is given by the solution of the Schr. eqn:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

where H is the operator associated with measurement of energy. H is called the Hamiltonian.

This postulate is rather explicit & detailed. Here is an alternate formulation:

Postulate 6'

Time evolution on $\mathcal{H}$ is represented by a continuously generated unitary transformation.

- We already know what a unitary transformation is. What about "continuously generated"?
- It means that there is a family of unitary transformations $\mathcal{U}(t)$ depending continuously on t, such that $\mathcal{U}(t=0) = \mathbb{1}$
- After some reflection, this postulate is obvious. We have assigned physical significance to the normalization of $|\psi\rangle$. So this normalization should not change as $|\psi\rangle$ evolves in time. If this is true of every state, the transformation

$$|\psi\rangle \xrightarrow[\mathcal{U}(t)]{} |\psi(t)\rangle$$ must be unitary.

- The simplest way to ~~construct~~ analyze a continuously generated unitary transformation is to examine an infinitesimal step, close to $\mathbb{1}$.

- For small t, we can write

$$\mathcal{U}(t) = \mathbb{1} + itG(t) + \mathcal{O}(t^2)$$

where G is some operator & we can neglect order t^2 terms if t is small enough.

- G is called the "generator" of $\mathcal{U}(t)$

- Also for T large + t small (some small step from some later time)

$$\mathcal{U}(T+t) = \left(1 + itG(t) + \mathcal{O}(t^2)\right)\mathcal{U}(T)$$
$$= \mathcal{U}(t)\,\mathcal{U}(T)$$

- In principle G can depend on the parameter t. However, for many cases, G is constant. Here we are interested in time translation, so statement that G is constant is statement that equations of motion of the universe are unchanging in time.

- To understand the relation between G & $\mathcal{U}(t)$ more clearly, let's work out the consequences of $\mathcal{U}(t)$ being unitary:

$$\mathcal{U}^\dagger(t)\,\mathcal{U}(t) = \mathbb{1}$$

for small t, $\mathcal{U}^\dagger(t) = 1 - itG^\dagger + O(t^2)$

$$\Rightarrow \mathcal{U}^\dagger(t)\,\mathcal{U}(t) = (1 - itG^\dagger + \ldots)(1 + itG + \ldots)$$
$$= 1 + it\left(G - G^\dagger\right) + O(t^2)$$

This must equal 1 for all orders of t.

So, looking at first order, we see

$$\mathcal{U}^\dagger \mathcal{U} = \mathbb{1} \iff G = G^\dagger$$

G is Hermitian.

* - So every observable $\mathcal{O}$ can be used to generate a unitary transformation on Hilbert space $\mathcal{H}$.

- We know a lot about Hermitian operators. In particular, we can diagonalize a Hermitian operator G & represent any state $|\psi\rangle$ as a linear combination of its eigenvectors:

$$|\psi\rangle = \sum_i \alpha_i |\psi_i\rangle, \text{ where } G|\psi_i\rangle = g_i |\psi_i\rangle$$

- This connection to Hermitian operator/observable clarifies the structure of the corresponding ~~with the choice to use eigenstates of G as basis~~ unitary transformation. - we can build a finite transformation from an infinitesimal one carried out a large number of times.

- For t finite now, we can divide it into N intervals so that t/N is small.

- Then $\mathcal{U}(t/N) \approx \mathbb{1} + i\frac{t}{N}G$

To recover $\mathcal{U}(t)$, we carry $\mathcal{U}(t/N)$ out N times:

$$\mathcal{U}(t) = \left[1 + i\frac{t}{N}G\right]^N \quad \text{in the limit } N \to \infty$$

Now use the formula

$$\lim_{N\to\infty} \left(1 + \lambda\frac{x}{N}\right)^N = e^{\lambda x},$$ (where λ can be an operator... strange at first)

Proof ~~to show it really works OK with operators in expo~~

(1) Taylor expand (in z) $(1+z)^\alpha = 1 + \frac{\alpha}{1!}z + \frac{\alpha(\alpha-1)}{2!}z^2 + \ldots$

$$\left(1 + \frac{\lambda x}{N}\right)^N = 1 + N\left(\frac{\lambda x}{N}\right) + \frac{N(N-1)}{2!}\left(\frac{\lambda x}{N}\right)^2 + \ldots$$

$$\xrightarrow[N\to\infty]{} 1 + (\lambda x) + \frac{1}{2!}(\lambda x)^2 + \ldots$$

$$= e^{\lambda x}$$

(2) $f_N(x) = \left(1 + \frac{\lambda x}{N}\right)^N$ obeys the differential equation

$$\frac{d}{dx} f_N(x) = \frac{\lambda}{\left(1 + \frac{\lambda x}{N}\right)} f_N(x) \quad \text{with} \quad f_N(0) = 1$$

$$\uparrow$$

$$\left(y = \left(1 + \frac{\lambda x}{N}\right) \qquad \frac{df_N}{dx} = \frac{df_N}{dy}\frac{dy}{dx} = N y^{N-1} \cdot \frac{\lambda}{N} = \frac{\lambda}{\left(1 + \frac{\lambda x}{N}\right)} f_N(x) \right)$$

As $N \to \infty$, this equation becomes

$$\frac{d}{dx} f(x) = \lambda f(x),$$ for which the solution is $f(x) = e^{\lambda x}$

Thus the unitary transformation generated by G is

$$\mathcal{U}(t) = e^{itG}$$

unitless

has units

We can interpret this expression in two equivalent ways:

(1) $e^{itG}|\psi\rangle = \left[1 + itG - \frac{1}{2!}(tG)^2 + \ldots\right]|\psi\rangle$

(operator in an exponential is just a sum like this)

(2) On an eigenvector of G: $e^{itG}|\psi_i\rangle = e^{itg_i}|\psi_i\rangle$

or on a general state: $|\psi\rangle = \sum_i \alpha_i |\psi_i\rangle$

$$e^{itG}|\psi\rangle = \sum \alpha_i e^{itg_i}|\psi_i\rangle$$

- So writing $\mathcal{U}(t)$ in terms of a Hermitian generator allows us to write explicit expressions for Postulate 6'.
- All this formalism applies to any continuously generated unitary transformation. Now think specifically about time translation on $\mathcal{H}$. Let G be the generator of this transformation.

- By thinking a bit, we can figure out what observable must be associated with G

- Say we start system in $|\psi_i\rangle$ such that

$$G|\psi_i\rangle = g_i|\psi_i\rangle$$

- Time evolution takes $|\psi_i\rangle \to |\psi(t)\rangle = U(t)|\psi_i\rangle$

$$= e^{+itG}|\psi_i\rangle$$

$$= e^{itg_i}|\psi_i\rangle$$

which is just a phase times $|\psi_i\rangle$.

$\Rightarrow$ If we start in a ~~definite~~ state with definite value of G, we stay in same definite value for all time. In other words, G is a conserved quantity.

- More generally, arbitrary matrix elements of G are conserved:

$$\langle \psi | G | \chi \rangle \rightarrow \langle \psi(t) | G | \chi(t) \rangle$$
$$= \langle e^{iGt}\psi_i | G | e^{iGt}\chi_i \rangle$$
$$= \langle \psi_i | e^{-iGt} G e^{iGt} | \chi_i \rangle$$
$$= \langle \psi_i | G | \chi_i \rangle \quad (G e^{iGt} = e^{iGt} G)$$

$$\Rightarrow \frac{d}{dt} \langle \psi^{(t)} | G | \chi^{(t)} \rangle = 0$$ for arbitrary states, not necessarily eigenstates of G

- So, whatever G is, it is a conserved quantity. Further, it is a scalar quantity, since it has to multiply t to get a number.
- There are very few conserved quantities in physics.
- In fact, there is only one conserved scalar, two conserved vectors (momentum + angular momentum).
- The conserved scalar is energy.
- Thus, the generator for $U(t)$ must be the energy operator!
- And we need a new constant with units $E \cdot t$ to make the exponent in e^{itG} unitless:

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

- A prediction of Planck's constant as well?

- But recall that in classical mechanics, conservation of energy is associated with time translation invariance. So, it is not surprising that this happens in QM as well.

- We have arrived at Postulate 6 from a more basic principle! (just postulating some things about Hilbert spaces & measurements & following them to logical conclusion)

- What about the sign in the exponent $e^{-\frac{iHt}{\hbar}}$?

- This is the sign we need to describe basic processes. E.g. $e^{i(kx-\omega t)}$, for $k>0$ & $E>0$, $\omega>0$, moves to right as $t\uparrow$. So, we need "$-$" sign to get wavepackets moving in right direction.

- (Note, this is not just a matter of reversing the direction of time. In QM, to do that you need to both take $i \to -i$ in that operator & change the initial state by $\psi \to \psi^*$)