Lecture 14

Some Basics on Quantum Mechanics

Let $\mathcal{H}$ be a complex Hilbert space. A quantum mechanical system on $\mathcal{H}$ is often modeled by a self-adjoint operator which we will denote by H. This operator $H^* = H$ is often called the Hamiltonian associated with this quantum system. Since H is self-adjoint, any eigenvalues of H are real. These eigenvalues, and more generally other elements in the spectrum of H, are often referred to as the allowed energies for the system. In this sense, the Hamiltonian H describes the total energy of the system.

Although for many quantum mechanical systems of interest the relevent Hamiltonians are unbounded self-adjoint operators, we will focus primarily on the case of bounded Hamiltonians. Note that, for spin systems, the Hilbert space is finite dimensional, and all self-adjoint operators are bounded.

The Schrödinger Perspective

Let H be a bounded selfadjoint operator on a complex Hilbert space $\mathcal{H}$. In this case, $H \in B(\mathcal{H})$ and so the Hamiltonian is an observable of the system.

One of the basic postulates of quantum mechanics is that the time evolution of the system is governed by the Schrödinger equation:

Given a bounded, self-adjoint operator H on $\mathcal{H}$ and a vector $\psi_0 \in \mathcal{H}$, the equation

$$i \frac{d}{dt} \psi(t) = H\psi(t) \qquad \text{with } \psi(0) = \psi_0$$

is the well-known Schrödinger equation.

__Note__: Here we work in units where Planck's constant $\hbar = 1$.

As is well-known, the unique solution of this linear differential equation is

$$\psi(t) = e^{-itH} \psi_0 \qquad \text{for all } t \in \mathbb{R}.$$

Here $t \in \mathbb{R}$ is thought of as time.

Of course, if $\psi : \mathbb{R} \to \mathbb{C}$ and $H \in \mathbb{R}$, the differential equation

$$\psi' = -iH\psi \quad \text{with } \psi(0) = \psi_0$$

is a simple linear, 1st order differential equation for an unknown complex-valued function ψ.

The solution is clearly

$$\psi(t) = e^{-itH}\psi_0 .$$

It is an interesting fact that the previous Hilbert space valued differential equation can also be solved, and moreover, the solution has the same form.

It is convenient to introduce notation for the family of operators $\{U_t\}_{t\in\mathbb{R}}$ with $U_t = e^{-itH}$ for all $t \in \mathbb{R}$.

<u>Note that:</u>

- $U_t \in B(\mathcal{H})$ for all $t \in \mathbb{R}$
- $U_t^* = U_{-t}$ and so $U_t^* U_t = \mathbb{1} = U_t U_t^*$ for all $t \in \mathbb{R}$.
- $U_{t+s} = U_t U_s = U_s U_t$ for all $t, s \in \mathbb{R}$

We conclude that: the family $\{U_t\}_{t\in\mathbb{R}}$ is a one-parameter group of unitary operators which describe the solution of the Schrödinger equation.

Note that:

As a consequence of unitarity,

$$\|\psi(t)\|^2 = \langle \psi(t), \psi(t) \rangle = \langle U_t \psi_0, U_t \psi_0 \rangle = \langle \psi_0, U_t^* U_t \psi_0 \rangle = \langle \psi_0, \psi_0 \rangle$$
$$= \|\psi_0\|^2$$

In words, the norm of the solution of Schrödinger's equation is preserved in time.

It is also clear that: For any $t, s \in \mathbb{R}$,

$$\psi(t+s) = U_{t+s}\psi_0 = U_t U_s \psi_0 = U_t \psi(s)$$

In words, the solution of the Schrödinger equation can be understood "incrementally" through the above expression.

As is clear from the manner in which we have introduced it, the solution of Schrödinger's equation describes for us how vectors in $\mathcal{H}$ (e.g. ψ_0) evolve in time under the influence of the Hamiltonian H.

This is "the Schrödinger perspective",

Another, equivalent, perspective was described by Heisenberg.

The Heisenberg Perspective

Let H be a bounded self-adjoint operator on $\mathcal{H}$ and take $\psi_0 \in \mathcal{H}$. For all $t \in \mathbb{R}$, denote by $\psi(t) \in \mathcal{H}$ the solution of Schrödinger's equation with $\psi(0) = \psi_0$.

Let us assume $\psi_0 \in \mathcal{H}$ is a unit vector and thus $\|\psi(t)\| = 1$ for all $t \in \mathbb{R}$ (by our previous discussion.).

Consider the vector state associated to $\psi(t)$:

$$\omega_{\psi(t)}(A) = \langle \psi(t), A\psi(t) \rangle \quad \text{for all } A \in \mathcal{B}(\mathcal{H}).$$

In this case,

$$\begin{aligned}
\omega_{\psi(t)}(A) = \langle \psi(t), A\psi(t) \rangle &= \langle U_t \psi_0, A U_t \psi_0 \rangle \\
&= \langle \psi_0, U_t^* A U_t \psi_0 \rangle \\
&= \omega_{\psi_0}(U_t^* A U_t).
\end{aligned}$$

In words, the vector state associated to $\psi(t)$ can be calculated in terms of the vector state associated to $\psi(0) = \psi_0$ if the observable is "time-evolved".

For any $t \in \mathbb{R}$, a map $\tau_t : B(\mathcal{H}) \to B(\mathcal{H})$ given by

$$\tau_t(A) = U_t^* A U_t = e^{itH} A e^{-itH} \qquad \text{for all } A \in B(\mathcal{H})$$

is called the Heisenberg dynamics (or Heisenberg time-evolution)

In this Heisenberg perspective (which is equivalent to Schrodinger's) the time-evolution of the quantum mechanical system under the influence of H is understood through the dynamic evolution of observables.

One checks that

- For each $t \in \mathbb{R}$, τ_t is an automorphism of $B(\mathcal{H})$.

In fact,

$$\tau_t(AB) = e^{itH} A B e^{-itH} = e^{itH} A e^{-itH} e^{itH} B e^{-itH}$$
$$= \tau_t(A)\, \tau_t(B)$$

i.e. τ_t preserves the product structure.

and

$$\tau_t(A)^* = \left(e^{itH} A e^{-itH}\right)^* = e^{itH} A^* e^{-itH} = \tau_t(A^*)$$

i.e. τ_t is a $*$-morphism from $B(\mathcal{H})$ to $B(\mathcal{H})$.

The remaining properties are easily checked ...

Given that each τ_t is an automorphism, our previous results imply that it preserves norm, i.e.

$$\|\tau_t(A)\| = \|A\| \qquad \text{for all } A \in B(\mathcal{H}).$$

(This is the analogue of unitarity of the Schrödinger evolution, but now on $B(\mathcal{H})$.)

These automorphisms also satisfy the group property:

$$\begin{aligned}
\tau_{t+s}(A) = e^{i(t+s)H} A e^{-i(t+s)H} &= U_{t+s}^* A U_{t+s} \\
&= (U_s U_t)^* A U_s U_t \\
&= U_t^* U_s^* A U_s U_t \\
&= \tau_t(\tau_s(A))
\end{aligned}$$

In this case, the family $\{\tau_t\}_{t\in\mathbb{R}}$ is a one-parameter group of automorphisms of $B(\mathcal{H})$.

It will also be useful for us to observe that this Heisenberg dynamics is the unique solution of a differential equation with values in $B(\mathcal{H})$.

To see this, let us introduce some notation.

To any $A, B \in \mathcal{B}(\mathcal{H})$, denote by $[A,B] \in \mathcal{B}(\mathcal{H})$, the <u>commutator of A and B</u> which is given by

$$[A,B] = AB - BA.$$

Note that if $[A,B] = 0$, then $AB - BA = 0$

i.e. $AB = BA$

and so A and B commute!

Let us now proceed with a formal calculation:

$$\frac{d}{dt}\tau_t(A) = \frac{d}{dt}\left(e^{itH} A e^{-itH}\right)$$

$$= iHe^{itH} A e^{-itH} - ie^{itH} A H e^{-itH}$$

$$= i e^{itH}(HA - AH)e^{-itH}$$

$$= i\,\tau_t([H,A]).$$

For the special case of $A = H$, we see that $\frac{d}{dt}\tau_t(H) = 0$.

Thus $\tau_t(H)$ is constant (in t).

$\Rightarrow \tau_t(H) = \tau_0(H) = H$ i.e. the Hamiltonian is time-invariant.

By the automorphism property of τ_t, one checks that

$$\tau_t([A,B]) = [\tau_t(A), \tau_t(B)] \quad \text{for any } A, B \in B(\mathcal{H}) \text{ and } t \in \mathbb{R}.$$

<u>Thus</u>

$$\frac{d}{dt}\tau_t(A) = i\,\tau_t([H,A])$$
$$= i\,[\tau_t(H), \tau_t(A)]$$
$$= i\,[H, \tau_t(A)].$$

One can show that the Heisenberg dynamics is the unique solution of the $B(\mathcal{H})$-valued differential equation

$$\frac{d}{dt} f(t) = i[H, f(t)] \quad \text{with} \quad f(0) = f_0 \in B(\mathcal{H}).$$

<u>Note:</u> $\tau_t(A)$ corresponds to the solution $f(t)$ above with initial condition $f_0 = A \in B(\mathcal{H})$.

As we will see, much of "basic quantum mechanics" requires an understanding of "calculus" for

- Hilbert space valued functions
- $B(\mathcal{H})$-valued functions.

We turn to this next