A Brief Overview from Dirac-von Neumann's Formulation of Quantum Mechanics to Schrödinger's Equation

Yifan Wei

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Abstract

Let me put this forward, this paper is more like a review of some basic ideas about quantum mechanics which I accessed a year ago, than a useless paper working on a problem that nobody cares about neither would last long.

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1 Introduction

1.1 Dirac-von Neumann's Axioms

1. The **state** of a system is a ray of vectors in a countably infinite dimensional Hilbert space $\mathcal{H}$ over the complex numbers.

   Usually we take the unit vector $|\Psi\rangle$ to represent the state Ψ. Where the Dirac's *bra-ket notation* has been used, i.e.

   the bra vector $\langle\Psi|$ for the conjugation of the ket vector $|\Psi\rangle$.

   And the inner product between two vectors $|\Psi_1\rangle$ and $|\Psi_2\rangle$ is denoted as

   $$\langle\Psi_1|\Psi_2\rangle,$$

which is a complex number with the property of *conjugal symmetry*

$$\langle \Psi_2 | \Psi_1 \rangle = \overline{\langle \Psi_1 | \Psi_2 \rangle}.$$

2. An **observable** of a system is a *self-adjoint* operator L. All values we can measure out of this observable are its *eigenvalues* (which are all *real*). Different unit eigenvectors represent different distinguishable (orthogonal) states, where the corresponding eigenvalue is the one you're expected to observe when the measurement is taking on this system at this state.

   If we measure a system at state $|\Psi\rangle$, the probability that the measure gives out the (eigen)value λ is

   $$|\langle \Psi_\lambda | \Psi \rangle|^2,$$

   where $|\Psi_\lambda\rangle$ is the unit eigenvector corresponding to λ. However, after one measurement, if the result turns out to be a certain μ, then the state of the system will be absolutely $|\Psi_\mu\rangle$, because quantum experiments are always **repeatable** and this is can be regard as a result of *entanglement* between the system and the machine we used to measure it.

3. The **expectation value** of an observable L on the system at state $|\Psi\rangle$ is

   $$\langle \Psi | L | \Psi \rangle.$$

   This can be seen as a combination of the **total probability formula** and the **spectrum theorem**.

1.2 Schrödinger Picture

In a Schrödinger picture, it's the state of system itself that evolves with time, rather than the observables. The evolution of a closed quantum system is brought about by a *unitary* operator, the **time evolution operator** $U(t)$, which has these properties

1. It doesn't change the orthogonality of states, which is from its definition, a unitary operator.

2. It shifts the state of a system to a *future* state, i.e.

   $$U(t)|\Psi(t_0)\rangle = |\Psi(t_0 + t)\rangle.$$

2 Some Basic Results

2.1 Schrödinger's Equation

Assuming some smooth conditions on the time evolution operator, we may derive the equation that governs the evolution of state. Suppose

$$U(t) = I + \frac{1}{i\hbar} H t + o(t),$$

where we've used the Landau's little o notation. The operator in front of t is assumed to be of this spectacular form is just for latter convenience.

Since $U(t)$ is unitary, we surely have

$$
\begin{aligned}
I = U^\dagger(t)U(t) &= \left(I - \frac{1}{i\hbar}H^\dagger t + (o(t))^\dagger\right)\left(I + \frac{1}{i\hbar}Ht + o(t)\right) \\
&= I + \frac{1}{i\hbar}(H - H^\dagger)t + o(t),
\end{aligned}
$$

where $\dagger$ means the adjoining operator. Cancelling I on both sides and divide them by t, we will find that

$$H = H^\dagger,$$

which means that H is a self-adjoint operator, after we letting t tend to 0.

On the other hand, we have

$$
\begin{aligned}
\lim_{s\to 0}\frac{1}{s}(|\Psi(t+s)\rangle - |\Psi(t)\rangle) &= \lim_{s\to 0}\frac{1}{s}(U(s) - I)|\Psi(t)\rangle \\
&= \frac{1}{i\hbar}H|\Psi(t)\rangle.
\end{aligned}
$$

Which is actually the famous (time-dependent) Schrödinger equation

$$\frac{\partial}{\partial t}|\Psi\rangle = \frac{1}{i\hbar}H|\Psi\rangle.$$

But we still don't know anything about H, except the fact that it is self-adjoint. So we can survey its eigenvalues and eigenvectors, and this lead us to this equation

$$H|\Psi\rangle = E|\Psi\rangle,$$

the time-independent Schrödinger equation, where E is a real number.

If we had all the eigenvalues E_k and eigenvectors $|\Psi_k\rangle$ of H, we can use the spectrum theorem to help us solve the time-dependent one. Because the eigenvectors $|\Psi_k\rangle$ form an orthogonal basis in $\mathcal{H}$, so we can evaluate the coordinates of $|\Psi\rangle$. Let

$$c_k(t) = \langle\Psi_k|\Psi(t)\rangle,$$

we got

$$|\Psi\rangle = \sum_k c_k(t)|\Psi_k\rangle.$$

Taking it into the time-dependent Schrödinger equation, we have

$$\sum_k \frac{\partial}{\partial t}c_k(t)|\Psi_k\rangle = \frac{1}{i\hbar}\sum_k c_k(t)H|\Psi_k\rangle = \frac{1}{i\hbar}\sum_k E_k c_k(t)|\Psi_k\rangle.$$

Thus

$$c_k(t) = \exp(tE/i\hbar)c_k(0), \qquad |\Psi(t)\rangle = \sum_k \exp(tE/i\hbar)c_k(0)|\Psi_k\rangle.$$

A little observation we can make now is that the possibility of find the system at each state remain unchanged as time evolving. Reminding us there's something conserved in time.

2.2 The Expectation Values

We can make use of this equation further, to the evolving of expectation values. Differentiating the representation of expectation value gives

$$\begin{aligned}\frac{\partial}{\partial t}\langle\Psi|L|\Psi\rangle &= \left(\frac{\partial}{\partial t}\langle\Psi|\right) L|\Psi\rangle + \langle\Psi|L\left(\frac{\partial}{\partial t}|\Psi\rangle\right) \\ &= -\frac{1}{i\hbar}\langle\Psi|HL|\Psi\rangle + \frac{1}{i\hbar}\langle\Psi|LH|\Psi\rangle \\ &= \frac{1}{i\hbar}\langle\Psi|LH - HL|\Psi\rangle,\end{aligned}$$

whcih is usually simplyfied to

$$\frac{\partial}{\partial t}\langle L\rangle = \frac{1}{i\hbar}\langle[L, H]\rangle,$$

where $[L, H] = LH - HL$ is called the commutator. This is like in the Hamiltonian mechanics where we have a similar formula

$$\frac{\partial}{\partial t}L = -\{L, H\},$$

where L is the phase space distribution and $\{\cdot,\cdot\}$ is the Poisson bracket, and H is the Hamiltonian of that system. I guess this is where physicists begin to believe quantum H is a similar thing which is the observable of **total energy**.