Observables, Hamiltonian, Schrödinger Equation

1 Observables

An observable is a physical quantity, such as energy, spin or position, that can be measured; think of a measuring device with a pointer from which you can read off a real number which is the outcome of the measurement. For a k-state quantum system, observables correspond to $k \times k$ hermitian matrices. Recall that a matrix M is hermitian iff $M^\dagger = M$. Since M is hermitian, it has an orthonormal set of eigenvectors $|\phi_j\rangle$ with real eigenvalues λ_j. If the quantum state of the system is $|\psi\rangle$, what is the outcome of the measurement M? To understand this, let us write $|\psi\rangle = a_0\phi_0 + \cdots + a_{k-1}\phi_{k-1}$ in the $\{|\phi_j\rangle\}$-basis. Now, the result of the measurement is λ_j (this is real number we read off our measurement device) with probability $|a_j|^2$. Moreover, the state of the system is reset to $|\phi_j\rangle$.

It should be clear how this description of a measurement corresponds to what we described earlier while expaining the measurement principle: there a measurement was specified by picking an orthonormal basis $\{|\phi_j\rangle\}$, and the measurement outcome was j with probability $|a_j|^2$. The sequence of real numbers λ_j simply provide a way of specifying what the pointer of the measurement device indicates for the j-th outcome. Moreover given any orthonormal basis $|\phi_j\rangle$ and the sequence of real numbers λ_j, we can reconstruct a hermitian matrix M as: $M = \sum_{j=0}^{k-1} \lambda_j |\phi_j\rangle\langle\phi_j|$; in the $\{|\phi_j\rangle\}$-basis this is just a diagonal matrix with the λ_js on the diagonal.

For example, if we wished to measure in the $|+\rangle, |-\rangle$-basis, with measurement results 1 and -1 respectively, then the corresponding operator is $M = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} - \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

One important observable of any quantum system is its energy; the corresponding hermitian matrix or operator is called the Hamiltonian. The eigenvectors of this operator are the states of the system with definite energy, and the eigenvectors are the numerical values of the energies of these eigenstates.

As we saw above, the outcome of the measurement M is probabilistic. Thus if M were the Hamiltonian of the system, we could ask for a given state ψ, "what is the expected energy of this state?" In our notation above, this expected value would be $\sum_{j=0}^{k-1} |a_j|^2 \lambda_j$. This is exactly the value of the bilinear form $\langle\psi|M|\psi\rangle$.

How much does the value of the energy of the state $|\psi\rangle$ vary from measurement to measurement? One way of estimating this is to talk about the variance, $Var(X)$ of the measurement outcome. Recall that $Var(X) = E(X^2) - E(X)^2$. So to compute the variance we must figure out $E(X^2)$, the expected value of the square of the energy. This expected value is $\sum_{j=0}^{k-1} |a_j|^2 \lambda_j^2$. This is exactly the value of the bilinear form $\langle\psi|M^2|\psi\rangle$.

So the variance of the measurement outcome $Var(X) = E(X^2) - E(X)^2 = \langle\phi|M^2|\phi\rangle - (\langle\phi|M|\phi\rangle)^2$.

2 Schrödinger's Equation

Schrödinger's equation is the most fundamental equation in quantum mechanics — it is the equation of motion which describes the evolution in time of the quantum state.

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

Here H is the Hamiltonian or energy operator, and $\hbar$ is a constant (called Planck's constant – for now we will simply select our units such that $\hbar = 1$,) To understand Schrödinger's equation, it is instructive to analyze what it tells us about the time evolution of the eigenstates of the Hamiltonian H. So let us assume that $\left|\psi(0)\right\rangle = \left|\phi_j\right\rangle$, an eigenvector of H with eigenvalue λ_j. Now by Schrödinger's equation, $\frac{d\left|\psi(0)\right\rangle}{dt} \propto H\left|\phi_j\right\rangle \propto \left|\phi_j\right\rangle$. Thus $\left|\psi(t)\right\rangle = a(t)\left|\phi_j\right\rangle$.

Substituting into Schrödinger's equation, we get: $i\frac{da(t)\left|\phi_j\right\rangle}{dt} = H\left|a(t)\phi_j\right\rangle$. Therefore $i\frac{da(t)}{dt}\left|\phi_j\right\rangle = a(t)\lambda_j\left|\phi_j\right\rangle$. $\Longrightarrow i\frac{da(t)}{a(t)} = \lambda_j dt$. Integrating both sides with respect to t: $i\ln a(t) = \lambda_j t$. Therefore $a(t) = e^{-i\lambda_j t}$, and $\left|\psi(t)\right\rangle = e^{-i\lambda_j t}\left|\phi_j\right\rangle$.

So each energy eigenstate $\left|\phi_j\right\rangle$ is left invariant over time, but its phase precesses at a rate proportional to its energy λ_j.

What about a general quantum state $\left|\psi(0)\right\rangle = \sum_j a_j\left|\phi_j\right\rangle$? By linearity, $\left|\psi(t)\right\rangle = \sum_j a_j e^{-i\lambda_j t}\left|\phi_j\right\rangle$.

We can write this as a matrix equation:

$$\left|\psi(t)\right\rangle = \begin{pmatrix} e^{-\frac{i}{\hbar}\lambda_1 t} & & 0 \\ & \ddots & \\ 0 & & e^{-\frac{i}{\hbar}\lambda_d t} \end{pmatrix} \begin{pmatrix} a_0 \\ \cdot \\ \cdot \\ a_d \end{pmatrix} = U(t)\left|\psi(0)\right\rangle$$

We have proved that if the Hamiltonian H is time independent, then Schrödinger's equation implies that the time evolution of the quantum system is unitary. Moreover, the time evolution operator $U(t)$ is diagonal in the basis of eigenvectors of H.

3 Why the Hamiltonian?

Let us try to understand why the energy operator governs the time evolution of the quantum state in Schrödinger's equation. We start with the unitary evolution axiom of quantum mechanics, which states that time evolution is given by a unitary operator U. Moreover, any unitary operator can be written as $U = e^{iM}$ where M is a hermitian matrix. [1]

Consider a "time independent situation", where the external conditions to which the system is subjected do not change in time. Let e^{iM} be the unitary operator corresponding to evolution for one unit of time. So the time evolution for two units of time is given by:

$$U(2) = U(1)U(1) = e^{iM}e^{iM} = e^{i2M}$$

In general, the time evolution for n units of time is given by $U(n) = e^{inM}$, and we can express this as

$$U(t) = e^{iMt}$$

Energy is probably the most important physical observable characterizing the system. We will now show why energy is intimately related to time evolution. The basic fact is that in physical situations in which the external conditions are unchanged in time, energy is conserved (if the external conditions change, the energy of the system can change; for example the system collides with an external particle. Of course, we can enlarge our definition of the "system" to include the external particle, and then the total energy is conserved).

[1] This follows from the fact that U has an orthonormal set of eigenvectors with complex eigenvalues $\{e^{i\theta}\}$. Let M be the hermitian matrix with the same eigenvectors and eigenvalues $\{\theta\}$.

First, we will see that if A is any observable that corresponds to a physical quantity that is conserved, then A commutes with M, the hermitian operator in Schrödinger's equation.

Let $|\psi\rangle$ be the initial state of the system, and $|\psi'\rangle = U|\psi\rangle = e^{iMt}|\psi\rangle$ be the state after an infinitesimal time interval t.
Since A corresponds to a conserved physical quantity, $\langle\psi'|A|\psi'\rangle = \langle\psi|A|\psi\rangle$.
i.e. $\langle\psi|U^\dagger AU|\psi\rangle = \langle\psi|A|\psi\rangle$.
Since this equation holds for every state $|\psi\rangle$, it follows that $U^\dagger AU = A$.
Substituting for U, we get
$LHS = e^{-iMt}Ae^{iMt} \approx (1-iMt)A(1+iMt) \approx 1-it[M,A]$
where $[M,A] = MA - AM$.
It follows that $[M,A] = 0$.

So any observable corresponding to a conserved quantity must commute with the operator M that describes the time evolution. Now, in addition to energy, there are situations where other physical quantities, such as momentum or angular momentum, are also conserved. These are in a certain sense "accidental" conservation relations — they may or may not hold. Energy however is always conserved. Hence the operator H cannot be just any operator that happens to commute with M, but must have some universal property. An intrinsic reason that H might commute with M is that $H = f(M)$. i.e. H is some function of M. Indeed any function of M commutes with M.

We now finish up by showing that if $H = f(M)$, it must necessarily be a linear function. Consider a quantum system consisting of two subsystems that do not interact with each other. Then if M_1 and M_2 are the time evolution operators corresponding to each subsystem, then $M_1 + M_2$ is the time evolution operator of the system (since the two subsystems do not interact). So the total energy of the system is $f(M_1 + M_2)$. On the other hand, since the two subsystems do not interact, the system hamiltonian, $H = H_1 + H_2 = f(M_1) + f(M_2)$. Hence $f(M_1 + M_2) = f(M_1) + f(M_2)$, and therefore f is a linear function $f(M) = \hbar M$, where $\hbar$ is a constant. So $H = \hbar M$ and $U(t) = e^{iHt/\hbar}$. Since $Ht/\hbar$ must be dimensionless, the constant $\hbar$ must have units of energy x time.