Chapter 3

Observables

3.1 Observables

An observable is an operator that corresponds to 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. What is the outcome of a measurement of the quantity represented by observable M on a quantum state $|\psi\rangle$? 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 must be some λ_j (this is the real number we read off our measurement device) with probability $|a_j|^2$. Moreover, the state of the system is collapsed to $|\phi_j\rangle$.

This description of a measurement relates to what we described earlier while explaining 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_j's on the diagonal.

For example, suppose we wish to measure a qubit in the $|+\rangle, |-\rangle$-basis, with measurement results 1 and -1 respectively. This corresponds to measur-

ing the observable

$$\begin{aligned} M &= (1)\,|+\rangle\langle+| + (-1)\,|-\rangle\langle-| \\ &= \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} - \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

By construction M has eigenvectors $|+\rangle$ and $|-\rangle$ with eigenvalues 1 and -1 respectively.

One important observable of any physical system is its energy; the corresponding hermitian matrix or operator is called the Hamiltonian, and is often denoted by $\hat{H}$. The eigenvectors of this operator are the states of the system with definite energy, and the eigenvalues are the numerical values of the energies of these eigenstates.

Consider, for example, two states ψ_1 and ψ_2 such that $\hat{H}\psi_1 = E_1\psi_2$ and $\hat{H}\psi_2 = E_2\psi_2$, where $E_1 \neq E_2$ (in quantum mechanical language this means that the *eigenvalues are non-degenerate*). Suppose we take 10^6 qubits prepared in state ψ_1 and measure the energy of each one and make a histogram. What does the histogram look like? See Figure 1(a).

Now suppose that we prepare 10^6 qubits in the state $\psi' = \sqrt{\frac{3}{5}}\psi_1 + \sqrt{\frac{2}{5}}\psi_2$, measure each of *their* energies, and make a histogram. How does it look? See Figure 1(b)

Ask yourself, is ψ' a state with well-defined energy? The answer is *NO*. Why? Because ψ' is not an eigenstate of the Hamiltonian operator. Let's check this:

$$\hat{H}\psi' = \hat{H}\left(\sqrt{\frac{3}{5}}\psi_1 + \sqrt{\frac{2}{5}}\psi_2\right) = \sqrt{\frac{3}{5}}E_1\psi_1 + \sqrt{\frac{2}{5}}E_2\psi_2$$

Does this equal (constant)$\times(\psi')$? No, because E_1 and E_2 are not equal. Therefore ψ' is not an eigenstate of the energy operator and has no well-defined energy.

Even though a given state $|\psi\rangle$ might not have a definite energy, we can still ask the question, "what is the expected energy of this state?" i.e. if we prepare a large number of systems each in the state $|\psi\rangle$, and then measure their energies, what is the average result? 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 $\langle\psi|\, M\, |\psi\rangle$. Returning to our example above, where $M = H$, this expected value is $\frac{3}{5}E_1 + \frac{2}{5}E_2$.

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, $\mathrm{var}(X)$ of the measurement outcome. Recall that

$$\mathrm{var}(X) = E(X^2) - E(X)^2.$$

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 for the state, $|\psi\rangle$ is

$$\mathrm{var}(X) = E(X^2) - E(X)^2 = \langle\psi| M^2 |\psi\rangle - (\langle\psi| M |\psi\rangle)^2.$$

Returning to our example above,

$$\langle\psi'| M^2 |\psi'\rangle = \sum_{j=0}^{k-1} |a_j|^2 \lambda_j^2 = \frac{3}{5}E_1^2 + \frac{2}{5}E_2^2.$$

The variance is therefore

$$\mathrm{var}(X) = \frac{3}{5}E_1^2 + \frac{2}{5}E_2^2 - (\frac{3}{5}E_1 + \frac{2}{5}E_2)^2.$$

Schrödinger's Equation

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

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. Let's assume we are given a quantum system whose state at time $t = 0$ is, $|\psi(0)\rangle = |\phi_j\rangle$, an eigenstate of the Hamiltonian with eigenvalue, λ_j. Plugging this into Schrödinger's equation,

$$\frac{d|\psi(0)\rangle}{dt} = -\frac{i}{\hbar}H|\phi_j\rangle = -\frac{i}{\hbar}\lambda_j|\phi_j\rangle$$

So let us consider a system that is in the state $|\psi\rangle$ at time $t = 0$ such that that $|\psi(0)\rangle = |\phi_j\rangle$, an eigenvector of H with eigenvalue λ_j. Now by Schrödinger's equation,

$$\frac{d\,|\psi(0)\rangle}{dt} = -H\,|\phi_j\rangle\,/\hbar = -i\lambda_j/\hbar\,|\phi_j\rangle\,.$$

Thus $|\psi(t)\rangle = a(t)\,|\phi_j\rangle$. Substituting into Schrödinger's equation, we get:

$$i\frac{da(t)\,|\phi_j\rangle}{dt} = H\,|a(t)\phi_j\rangle = a(t)\lambda_j\,|\phi_j\rangle\,.$$

Thus $i\hbar\frac{da(t)}{a(t)} = \lambda_j dt$. Integrating both sides with respect to t: $i\hbar \ln a(t) = \lambda_j t$. Therefore $a(t) = e^{-i\lambda_j t/\hbar}$, and $|\psi(t)\rangle = e^{-i\lambda_j t/\hbar}\,|\phi_j\rangle$.

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

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

In the basis of eigenstates of H, we can write this as a matrix equation:

$$|\psi(t)\rangle = \begin{pmatrix} e^{-\frac{i}{\hbar}\lambda_1 t} & & 0 \\ & \ddots & \\ 0 & & e^{-\frac{i}{\hbar}\lambda_d t} \end{pmatrix} \begin{pmatrix} a_0 \\ \vdots \\ a_{k-1} \end{pmatrix} = U(t)\,|\psi(0)\rangle$$

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, and can be written as $U(t) = e^{\frac{-iHt}{\hbar}}$.

Returning to our running example, suppose $\psi(x, t = 0) = \psi_1(x)$ where $\hat{H}\psi_1 = E_1\psi_1(x)$. What is $\psi(x, t \neq 0)$? The answer is,

$$\psi(x,t) = \psi_1(x)e^{-iE_1 t/\hbar}$$

But what if $\psi(x, t = 0) = \psi' = \sqrt{\frac{3}{5}}\psi_1 + \sqrt{\frac{2}{5}}\psi_2$? What's $\psi(x, t \neq 0)$ in this case? The answer then becomes,

$$\psi(x,t) = \sqrt{\frac{3}{5}}\psi_1 e^{-iE_1 t/\hbar} + \sqrt{\frac{2}{5}}\psi_2 e^{-iE_2 t/\hbar}$$

Each different piece of the wavefunction with differnt well-defined energy dances to its own little drummer. Each piece *spins* at frequency proportional to its energy.

Conservation Laws and the Hamiltonian

Energy is typically the most important physical observable characterizing any system. You might still wonder, "why is energy so intimately related to the time evolution of a quantum system?" In this section we will try to answer this question. The answer is related to a fundamental physical principle, namely the conservation of energy.

We start by assuming that the time evolution of the state $|\psi\rangle$ in Schrödinger's equation is governed by some arbitrary hermitian operator M, or equivalently that the evolution of the system is given by some unitary transformation $U = e^{-iMt}$ (with a little bit of work this can be shown to follow from the third axiom of quantum mechanics in the "time independent situation", where the external conditions the system is subject to do not change over time). So our question reduces to asking, why is the operator M necessarily the energy operator?

To see this, we must first show that if A is any observable corresponding to a physical quantity that is conserved in time, then A commutes with M (as defined above).

Let $|\psi\rangle$ be the initial state of some physical 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
$LHS = e^{-iMt}Ae^{iMt} \approx (1 - iMt)A(1 + iMt) \approx A - it[M, A]$
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 for all physical systems. An intrinsic reason that H might commute with M is that $H = f(M)$. i.e. H is some function of M. Since any function of M commutes with M we now assume that $H = f(M)$.

The next critical point to show is that if $H = f(M)$, then f must necessarily be a linear function. Consider a quantum system consisting of two subsystems that do not interact with each other. 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.