

Notice the dagger that indicates Hermitian conjugation. Now, let's plug Eqs. 4.1 and 4.3 into Eq. 4.2:

$$\langle \Psi(0) | \mathbf{U}^\dagger(t) \mathbf{U}(t) | \Phi(0) \rangle = 0. \quad (4.4)$$

To examine the consequences of this equation, consider an orthonormal basis of vectors $|i\rangle$. Any basis will do. The orthonormality is expressed in equation form as

$$\langle i | j \rangle = \delta_{ij},$$

where δ_{ij} is the usual Kronecker symbol.

Next, let's take $|\Phi(0)\rangle$ and $|\Psi(0)\rangle$ to be members of this orthonormal basis. Substituting into Eq. 4.4 gives

$$\langle i | \mathbf{U}^\dagger(t) \mathbf{U}(t) | j \rangle = 0 \quad (i \neq j)$$

whenever i and j are not the same. On the other hand, if i and j are the same, then so are the output vectors $\mathbf{U}(t)|i\rangle$ and $\mathbf{U}(t)|j\rangle$. In that case, the inner product between them should be 1. Therefore, the general relation takes the form

$$\langle i | \mathbf{U}^\dagger(t) \mathbf{U}(t) | j \rangle = \delta_{ij}.$$

In other words, the operator $\mathbf{U}^\dagger(t) \mathbf{U}(t)$ behaves like the unit operator I when it acts between any members of a basis set. From here it is an easy matter to prove that $\mathbf{U}^\dagger(t) \mathbf{U}(t)$ acts like the unit operator I when it acts on any state. An operator \mathbf{U} that satisfies

$$\mathbf{U}^\dagger \mathbf{U} = I$$

is called *unitary*. In physics lingo, *time evolution is unitary*.

Unitary operators play an enormous role in quantum mechanics, representing all sorts of transformations on the state-space. Time evolution is just one example. Thus, we conclude this section with a fifth principle of quantum mechanics:

- Principle 5: The evolution of state-vectors with time is unitary.

Exercise 4.1: Prove that if \mathbf{U} is unitary, and if $|A\rangle$ and $|B\rangle$ are any two state-vectors, then the inner product of $\mathbf{U}|A\rangle$ and $\mathbf{U}|B\rangle$ is the same as the inner product of $|A\rangle$ and $|B\rangle$. One could call this the *conservation of overlaps*. It expresses the fact that the logical relation between states is preserved with time.

4.5 The Hamiltonian

In the study of classical mechanics, we became familiar with the idea of an incremental change in time. Quantum mechanics is no different in this respect: we may build up finite time intervals by combining many infinitesimal intervals. Doing so will lead to a differential equation for the evolution of the state-vector. To that end, we replace the time interval t with an infinitesimal time interval ϵ and consider the time-evolution operator for this small interval.

There are two principles that go into the study of incremental changes. The first principle is unitarity:

$$\mathbf{U}^\dagger(\epsilon)\mathbf{U}(\epsilon) = I. \quad (4.5)$$

The second principle is continuity. This means that the state-vector changes smoothly. To make this precise, first consider the case in which ϵ is zero. It should be obvious that in this case the time-evolution operator is merely the unit operator I . Continuity means that when ϵ is very small, $\mathbf{U}(\epsilon)$ is close to the unit operator, differing from it by something of order ϵ . Thus, we write

$$\mathbf{U}(\epsilon) = I - i\epsilon\mathbf{H}. \quad (4.6)$$

You may wonder why I put a minus sign and an i in front of \mathbf{H} . These factors are completely arbitrary at this stage. In other words, they are a convention that has no content. I used them with an eye toward the future, when we will recognize \mathbf{H} as something familiar from classical physics.

We will also need an expression for \mathbf{U}^\dagger . Remembering that Hermitian conjugation requires the complex conjugation of coefficients, we find that

$$\mathbf{U}^\dagger(\epsilon) = I + i\epsilon\mathbf{H}^\dagger. \quad (4.7)$$

Now we plug Eqs. 4.6 and 4.7 into the unitarity condition of Eq. 4.5:

$$(I + i\epsilon\mathbf{H}^\dagger)(I - i\epsilon\mathbf{H}) = I.$$

Expanding to first order in ϵ , we find

Don't Understand $\rightarrow \mathbf{H}^\dagger - \mathbf{H} = 0$

or, in a format that is more illuminating,

$$\mathbf{H}^\dagger = \mathbf{H}. \quad (4.8)$$

This last equation expresses the unitarity condition. But it also says that \mathbf{H} is a Hermitian operator. This has great significance. We can now say that \mathbf{H} is an observable, and has a complete set of orthonormal eigenvectors and eigenvalues. As we proceed, \mathbf{H} will become a very familiar object, namely the *quantum Hamiltonian*. Its eigenvalues are the values that would result from measuring the energy of a quantum system. Exactly why we identify \mathbf{H} with the classical concept of a Hamiltonian, and its eigenvalues with energy, will become clear shortly.

Let's return now to Eq. 4.1 and specialize it to the infinitesimal case $t = \epsilon$. Using Eq. 4.6, we find

$$|\Psi(\epsilon)\rangle = |\Psi(0)\rangle - i\epsilon\mathbf{H}|\Psi(0)\rangle.$$

This is just the kind of equation that we can easily turn into a differential equation. First, we transpose the first term on the right side over to the left side, and then divide by ϵ :

$$\frac{|\Psi(\epsilon)\rangle - |\Psi(0)\rangle}{\epsilon} = -i\mathbf{H}|\Psi(0)\rangle.$$

If you remember your calculus (see *Volume I* for a quick review), you'll recognize that the left-hand side of this equation looks exactly like the definition of a derivative. If we take the limit as $\epsilon \rightarrow 0$, it becomes the time derivative of the state-vector:

$$\frac{\partial|\Psi\rangle}{\partial t} = -i\mathbf{H}|\Psi\rangle. \quad (4.9)$$

We originally set things up so that the time variable was zero, but there was nothing special about $t = 0$. Had we chosen another time and done the same thing, we would have gotten exactly the same result, namely, Eq. 4.9. This equation tells us how the state-vector changes: if we know the state-vector at one instant, the equation tells us what it will be at the next. Eq. 4.9 is important enough to have a name. It is called the *generalized Schrödinger equation*, or more commonly, the *time-dependent Schrödinger equation*. If we know the Hamiltonian, it tells us how the state of an undisturbed system evolves with time. Art likes to call this state-vector *Schrödinger's Ket*. He even wanted to render the Greek symbol with little whiskers,¹ but I had to draw the line somewhere.

4.6 What Ever Happened to \hbar ?

I'm sure you have all heard of Planck's constant. Planck himself called it h and gave it a value of about $6.6 \times 10^{-34} \text{ kg m}^2 / \text{s}$.

¹OK, not really.

Later generations redefined it, dividing by a factor of 2π and calling the result \hbar :

$$\hbar = \frac{h}{2\pi} = 1.054571726 \dots \times 10^{-34} \text{ kg m}^2 / \text{s}.$$

Why divide by 2π ? Because it saves us from having to write 2π in lots of other places. Considering the importance of Planck's constant in quantum mechanics, it seems a little odd that it hasn't come up yet. We're going to correct that now.

In quantum mechanics, as in classical physics, the Hamiltonian is the mathematical object that represents the energy of a system. This raises a question that, if you are very alert, may have been a source of confusion. Take a good look at Eq. 4.9. It doesn't make dimensional sense. If you ignore $|\Psi\rangle$ on both sides of the equation, the units on the left side are inverse time. If the quantum Hamiltonian is really to be identified with energy, then the units on the right side are energy. Energy is measured in units of joules, or $\text{kg} \cdot \text{m}^2 / \text{s}^2$. Evidently, I've been cheating a little bit. The resolution of this dilemma involves \hbar , a universal constant of nature, which happens to have units of $\text{kg} \cdot \text{m}^2 / \text{s}$. A constant with these units is exactly what we need to make Eq. 4.9 consistent. Let's rewrite it with Planck's constant inserted in a way that makes it dimensionally consistent:

$$\hbar \frac{\partial|\Psi\rangle}{\partial t} = -i\mathbf{H}|\Psi\rangle. \quad (4.10)$$

Why is it that \hbar is such a ridiculously small number? The answer has much more to do with biology than with physics.