Chapter 10

Time Evolution

So far, we have been discussing *kinematics*—the description of a physical system. We will have more to say about kinematics this semester and next. But now the time has come to introduce *dynamics*—how a physical system evolves in time.

One of the invariances of any isolated physical system is the freedom to change the origin of time. Let us imagine a small (*infinitesimal*) change in the time variable (time "coordinate"):

$$t \to \bar{t} = t - \delta t, \quad \delta t = \text{constant}. \tag{10.1}$$

In going from t to $\bar{t}$, the origin of time is shifted *forward* by an amount δt. Under such a change in the time parameter, states and operators do not change. However, we want to introduce *new* states and *new* operators which have the same properties relative to the *new* time coordinate as the old states and operators had relative to the old time coordinate t:

$$t \text{ coordinate}: \quad X, \quad |\,\rangle, \quad \langle\,|, \tag{10.2a}$$

$$\bar{t} \text{ coordinate}: \quad \overline{X}, \quad \overline{|\,\rangle}, \quad \overline{\langle\,|}. \tag{10.2b}$$

The new states and operators have the same inter-relations as the old states and operators; therefore, the two sets are related by a *unitary transformation*:

$$\overline{X} = U^{-1}XU, \quad U^{-1} = U^\dagger, \quad \overline{|\,\rangle} = U^\dagger|\,\rangle, \quad \overline{\langle\,|} = \langle\,|U. \tag{10.3}$$

What can we say about the unitary operator here? If $\delta t = 0$, the change in the states and operators is zero, so $U = 1$. If $\delta t \neq 0$ but very small, U must differ infinitesimally from 1. We therefore write

$$U = 1 - \frac{i}{\hbar}\delta t\, H. \tag{10.4}$$

We'll see in a moment why it's convenient to have the $-i/\hbar$ factor. What are the properties of the operator H? U must be unitary:

$$1 = UU^\dagger = \left(1 - \frac{i}{\hbar}\delta t H\right)\left(1 + \frac{i}{\hbar}\delta t H^\dagger\right) = 1 - \frac{i}{\hbar}\delta t(H - H^\dagger) + O(\delta t^2). \tag{10.5}$$

Since δt is infinitesimial, we will omit the term of order δt^2. We must concude that

$$H = H^\dagger, \quad H \text{ is Hermitian.} \tag{10.6}$$

This is why the i was put in front of the $\delta t\, H$ term.

Therefore, we suspect that H must represent a physical property. We will see that it corresponds to the energy of the system; we will call H the *energy operator* or the *Hamiltonian*. Certainly, H has the right units to be an energy, since the units of $\hbar$ are energy times time.

What happens if the time displacement is not infinitesimal? We recognize that the above form corrsponds to the first two terms in the Taylor series for

$$U = e^{-itH/\hbar}. \tag{10.7}$$

Since this is indeed a unitary operator, this is indeed the correct extrapolation.

A *dynamical variable* is an operator, characterizing in part a dynamical system, which changes as time evolves. An example we've seen in this course is the angular momentum $\mathbf{J}$. Let $v(t)$ be some dynamical variable. What happens under an infinitesimal change in the time origin, given by Eq. (10.1)?

$$v(t) = v(\bar{t} + \delta t) = \overline{v}(\bar{t}), \tag{10.8}$$

where $\overline{v}$ is the new (transformed) variable: by definition, the new variable at the new time is the old variable at the old time. This is what we mean by saying that the new operators have the same properties relative to the new time coordinate as the old operators had relative to the old time coordinate. Simply changing the name of the coordinate, we have

$$\overline{v}(t) = v(t + \delta t) = v(t) + \delta t \frac{d}{dt} v(t) = v(t) - \delta v(t), \tag{10.9}$$

where $\delta v(t)$ is just the change in the operator at the same value of the time coordinate,

$$\delta v(t) = v(t) - \overline{v}(t). \tag{10.10}$$

On the other hand, we can compute δv from the unitary operator U:

$$\begin{aligned} \overline{v}(t) &= U^\dagger v(t) U = \left(1 + \frac{i}{\hbar}\delta t\, H\right) v(t) \left(1 - \frac{i}{\hbar}\delta t\, H\right) \\ &= v(t) + \frac{1}{i\hbar}\left[v(t)\, H\, \delta t - H\, \delta t\, v(t)\right]. \end{aligned} \tag{10.11}$$

It is convenient to introduce a new notation, the *commutator* of two operators:

$$[A, B] \equiv AB - BA. \tag{10.12}$$

Then

$$\delta v(t) = -\delta t \frac{d}{dt} v(t) = -\delta t \frac{1}{i\hbar}[v(t), H], \tag{10.13}$$

or

$$\frac{d}{dt}v(t) = \frac{1}{i\hbar}[v(t), H]. \tag{10.14}$$

Sometimes we deal with functions which besides depending on dynamical variables, make *explicit* reference to the time parameter as well:

$$F(v(t), t). \tag{10.15}$$

Under the above unitary transformation,

$$\begin{aligned}\overline{F} &= U^{-1}F(v(t),t)U = F(U^{-1}v(t)U, t) \\ &= F(\overline{v}(t), t),\end{aligned} \tag{10.16}$$

since the numerical coordinate t is not altered by a unitary transformation, and algebraic relations are preserved by unitary transformations. But directly,

$$\begin{aligned}U^{-1}FU &= \left(1 + \frac{i}{\hbar}\delta t\, H\right) F \left(1 - \frac{i}{\hbar}\delta t\, H\right) \\ &= F(v(t), t) + \frac{1}{i\hbar}[F, H\,\delta t].\end{aligned} \tag{10.17}$$

Then, from the definition of the derivative,

$$\frac{F(\overline{v}(t), t) - F(v(t), t)}{\delta t} = \frac{F(v(t+\delta t), t) - F(v(t), t)}{\delta t}, \tag{10.18}$$

we see that

$$\frac{d}{dt}F(v(t), t) - \frac{\partial}{\partial t}F(v(t), t) = \frac{1}{i\hbar}\left[F(v(t), t), H\right], \tag{10.19}$$

where the second term appears because under a unitary transformation the explicit time dependence is not changed. That is, the total derivative acts on both $v(t)$ and t, so the partial derivative removes that part of the total time derivative that comes from the explicit appearance of t in F. Thus

$$\frac{d}{dt}F = \frac{\partial}{\partial t}F + \frac{1}{i\hbar}[F, H]. \tag{10.20}$$

The commutator induces the time change in the dynamical variables; the partial derivative takes care of any explicit time dependence. These equations (10.14) and (10.20) are called the *Heisenberg equations of motion.*

Now, what about the states? How do state vectors evolve in time? Suppose we have a state specified by the value of a dynamical variable $v(t)$, v':

$$\langle v', t| \tag{10.21}$$

represents a state in which, at time t, $v(t)$ has the value v':

$$\langle v', t|v(t) = \langle v', t|v'. \tag{10.22}$$

Under the time displacement, the corresponding operator transformation is

$$v(t) \to \overline{v}(t) = v(t + \delta t) = U^{-1} v(t) U. \tag{10.23}$$

The corresponding transformation of the states is

$$\overline{\langle v', t|} = \langle v', t| U. \tag{10.24}$$

This is the state in which $\overline{v}(t)$ has the value v':

$$\begin{aligned} \overline{\langle v', t|}\overline{v}(t) &= \langle v', t| U U^{-1} v(t) U = \langle v', t| v(t) U = v' \langle v', t| U \\ &= \overline{\langle v', t|} v', \end{aligned} \tag{10.25}$$

as we expect. This is just the statement that under a unitary transformation, the eigenvalues of an operator do not change. Now recognize that $\overline{\langle v', t|}$ is the state in which $v(t + \delta t|$ has the value v' Therefore,

$$\overline{\langle v', t|} = \langle v', t + \delta t|; \tag{10.26}$$

it is the state which has the same properties at the time $t + \delta t$ as $\langle v', t|$ did at time t. Then

$$\langle v', t + \delta t| = \langle v', t| \left(1 - \frac{i}{\hbar} \delta t \, H \right), \tag{10.27}$$

where the unitary transformation relates analogous states at different times. Therefore,

$$i\hbar \frac{\langle v', t + \delta t| - \langle v', t|}{\delta t} = \langle v', t| H, \tag{10.28}$$

so in the limit $\delta t \to 0$,

$$i\hbar \frac{\partial}{\partial t} \langle v', t| = \langle v', t| H. \tag{10.29}$$

To get the corresponding statement for right vectors, we simply take the adjoint:

$$-i\hbar \frac{\partial}{\partial t} |v', t\rangle = H |v', t\rangle. \tag{10.30}$$

This is Schrödinger's equation, which governs the time evolution of states. (The partial derivative symbols in Eqs. (10.29) and (10.30) means only that v' is not being changed.)

We know that under unitary transformations, numbers do not change. Consider the matrix element

$$\begin{aligned} \langle v', t| F(t) |v'', t\rangle &= \overline{\langle v', t|}\overline{F}(t)\overline{|v'', t\rangle} \\ &= \langle v', t + \delta t| F(t + \delta t) |v'', t + \delta t\rangle, \end{aligned} \tag{10.31}$$

supposing that F is *not an explicit function of the time*. Therefore,

$$\langle v', t| F(t) |v'', t\rangle \tag{10.32}$$

is independent of the time, or

$$\frac{d}{dt}\langle v', t|F(t)|v'', t\rangle = 0. \tag{10.33}$$

Let's check this by using the equations of motion,

$$\begin{aligned}\frac{d}{dt}\langle v', t|F(t)|v'', t\rangle &= \langle v', t|\frac{1}{i\hbar}HF(t)|v'', t\rangle + \langle v', t|F(t)\frac{1}{-i\hbar}H|v'', t\rangle \\ &+ \langle v', t|\frac{1}{i\hbar}[F(t), H]|v'', t\rangle = 0.\end{aligned} \tag{10.34}$$

How does the energy operator depend on time?

$$\frac{dH}{dt} = \frac{\partial}{\partial t}H + \frac{1}{i\hbar}[H, H] = \frac{\partial}{\partial t}H, \tag{10.35}$$

so if H does not explicitly depend on time, which will be true if we're dealing with a self-contained or isolated system,

$$H = \text{ constant}; \tag{10.36}$$

in the language of classical mechanics, H is a constant of the motion.

How do we translate Schrödinger's equation to wavefunctions? Let

$$\langle a', t| \tag{10.37}$$

be a state in which the physical property, i.e., the dynamical variable, $A(t)$ has the value a' (we continue to suppose for simplicity that A completely characterizes the system)

$$\langle a', t|A(t) = \langle a', t|a'. \tag{10.38}$$

Let $|\ \rangle$ be an arbitrary state. The probability amplitude of finding the system in the state $\langle a', t|$, that is, of finding $A(t) = a'$, is the wavefunction

$$\psi(a', t) = \langle a', t|\ \rangle. \tag{10.39}$$

Now using Schrödinger's equation for states,

$$i\hbar\frac{\partial}{\partial t}\langle a', t|\ \rangle = \langle a'|H|\ \rangle. \tag{10.40}$$

If, in addition, $|\ \rangle = |E\rangle$ is an energy eigenstate,

$$H|E\rangle = E|E\rangle, \tag{10.41}$$

where E is the numerical value of the energy of that state, Schrödinger's equation becomes

$$i\hbar\frac{\partial}{\partial t}\langle a', t|E\rangle = E\langle a', t|E\rangle, \tag{10.42}$$

or

$$i\hbar\frac{\partial}{\partial t}\psi_E(a', t) = E\psi_E(a', t), \tag{10.43}$$

which is the Schrödinger equation for a wavefunction corresponding to a state of definite energy. The solution to this equation is immediate:

$$\psi_E(a', t) = e^{-iEt/\hbar}\psi_E(a', 0). \tag{10.44}$$

A state of definite energy has a wavefunction of constant magnitude, and a phase which oscillates in time with frequency

$$\omega = \frac{E}{\hbar}, \quad E = \hbar\omega. \tag{10.45}$$

Such states are called *stationary states*, since only the phase varies. The dynamical problem for a stationary state is to solve the eigenvalue equation

$$H|E\rangle = E|E\rangle, \tag{10.46}$$

for the states $|E\rangle$ and the energies E, which is sometimes, rather erroneously, called the "time-independent Schrödinger equation."

10.1 Spin-1/2

Suppose we now ask a dynamical question for spin 1/2. An atom with a definite value of the spin along the z axis, $\frac{\hbar}{2}\sigma_z'$, enters a region of magnetic field $\mathbf{B}$ oriented along the z' axis axis (note that we do not call the magnetic field $\mathbf{H}$ to avoid confusion with the Hamiltonian); as usual, the angle between the z direction and the z' direction is called θ. After a time t, what is the probability of finding the atom in the same state as originally; and what is the probability of finding it in the other state?

We want to compute the probability amplitude

$$\langle\sigma_z'', t|\sigma_z', 0\rangle, \tag{10.47}$$

the transition amplitude between the initial state $|\sigma_z', 0\rangle$ and the final state $|\sigma_z'', t\rangle$. The latter is the state in which $\sigma_z(t)$ has the value σ_z''. The probability amplitude satisfies

$$i\hbar\frac{\partial}{\partial t}\langle\sigma_z'', t|\sigma_z', 0\rangle = \langle\sigma_z'', t|H|\sigma_z', 0\rangle, \tag{10.48}$$

where

$$H = -\boldsymbol{\mu}\cdot\mathbf{B} = -\gamma\frac{\hbar}{2}\sigma_{z'}B. \tag{10.49}$$

One way of proceeding is to insert a complete set of σ_z states at time t:

$$\langle\sigma_z'', t|H|\sigma_z', 0\rangle = \sum_{\sigma_z'''}\langle\sigma_z'', t|H|\sigma_z''', t\rangle\langle\sigma_z''', t|\sigma_z', 0\rangle, \tag{10.50}$$

so if we write

$$\psi_{\sigma_z'}(\sigma_z'', t) = \langle\sigma_z'', t|\sigma_z', 0\rangle, \tag{10.51}$$

we have the matrix equation

$$i\hbar\frac{\partial}{\partial t}\psi_{\sigma'_z} = -\gamma\frac{\hbar}{2}B\sigma_{z'}\psi_{\sigma'_z}, \tag{10.52}$$

where, as seen in Eq. (8.32),

$$\sigma_{z'} = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}. \tag{10.53}$$

Thus, we obtain the matrix version of Schrödinger's equation

$$i\frac{\partial}{\partial t}\psi_{\sigma'_z} = -\omega\sigma'_z\psi_{\sigma'_z}, \quad \omega = \frac{1}{2}\gamma B. \tag{10.54}$$

Written in terms of components, this reads

$$i\frac{\partial}{\partial t}\begin{pmatrix} \psi(+) \\ \psi(-) \end{pmatrix} = -\omega\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}\begin{pmatrix} \psi(+) \\ \psi(-) \end{pmatrix}, \tag{10.55}$$

or the homogeneous system of equations,

$$i\frac{\partial}{\partial t}\psi(+) = -\omega\left(\cos\theta\psi(+) + \sin\theta e^{-i\phi}\psi(-)\right), \tag{10.56a}$$

$$i\frac{\partial}{\partial t}\psi(-) = -\omega\left(\sin\theta e^{i\phi}\psi(+) - \cos\theta\psi(-)\right). \tag{10.56b}$$

The way to solve this matrix equation is to note that $\psi_{\sigma'_z}$ must be a linear combination of the eigenfunctions $\psi_{\pm z'}$, Eqs. (8.45) and (8.52),

$$\psi_{+z'} = \begin{pmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{pmatrix}, \tag{10.57a}$$

$$\psi_{-z'} = \begin{pmatrix} -\sin\frac{\theta}{2}e^{-i\phi/2} \\ \cos\frac{\theta}{2}e^{i\phi/2} \end{pmatrix}, \tag{10.57b}$$

which satisfy the eigenvalue equations

$$\sigma_{z'}\psi_{\pm z'} = \pm\psi_{\pm z'}. \tag{10.58}$$

Thus we write, in terms of time-dependent coefficients,

$$\psi_{\sigma'_z}(t) = \alpha_+(t)\psi_{+z'} + \alpha_-(t)\psi_{-z'}, \tag{10.59}$$

and the Schrödinger equation (10.54) becomes

$$\begin{aligned} i\frac{\partial}{\partial t}\psi_{\sigma'_z} &= i\frac{d}{dt}\alpha_+(t)\psi_{+z'} + i\frac{d}{dt}\alpha_-(t)\psi_{-z'} \\ &= -\omega\left[\alpha_+(t)\psi_{+z'} - \alpha_-(t)\psi_{-z'}\right]. \end{aligned} \tag{10.60}$$

Now since $\psi_{+z'}$, $\psi_{-z'}$ are independent, indeed orthogonal, we must have

$$i\frac{d}{dt}\alpha_+(t) = -\omega\alpha_+(t), \quad i\frac{d}{dt}\alpha_-(t) = \omega\alpha_-(t), \tag{10.61}$$

which have the solutions

$$\alpha_+(t) = e^{i\omega t}\alpha_+(0), \quad \alpha_-(t) = e^{-i\omega t}\alpha_-(0). \tag{10.62}$$

We determine the constants $\alpha_\pm(0)$ from

$$\psi_{\sigma'_z}(0) = \alpha_+(0)\psi_{+z'} + \alpha_-(0)\psi_{-z'}. \tag{10.63}$$

If the initial state is "spin up," $\sigma'_z = +1$, this reads

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \alpha_+(0)\begin{pmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{pmatrix} + \alpha_-(0)\begin{pmatrix} -\sin\frac{\theta}{2}e^{-i\phi/2} \\ \cos\frac{\theta}{2}e^{i\phi/2} \end{pmatrix}, \tag{10.64}$$

or

$$1 = \left[\alpha_+(0)\cos\frac{\theta}{2} - \alpha_-(0)\sin\frac{\theta}{2}\right]e^{-i\phi/2}, \tag{10.65a}$$

$$0 = \left[\alpha_+(0)\sin\frac{\theta}{2} + \alpha_-(0)\cos\frac{\theta}{2}\right]e^{+i\phi/2}, \tag{10.65b}$$

The last equation implies

$$\alpha_+(0) = \beta\cos\frac{\theta}{2}, \quad \alpha_-(0) = -\beta\sin\frac{\theta}{2}, \tag{10.66}$$

and then the first equation here implies

$$1 = \beta e^{-i\phi/2}, \quad \beta = e^{i\phi/2}. \tag{10.67}$$

Thus the wavefunction is

$$\psi_{+z}(t) = e^{i\omega t}\cos\frac{\theta}{2}e^{i\phi/2}\psi_{+z'} - e^{-i\omega t}\sin\frac{\theta}{2}e^{i\phi/2}\psi_{-z'}. \tag{10.68}$$

What did we do here? We wrote, inserting a complete set of z' states,

$$\begin{aligned}\psi_{\sigma'_z}(\sigma''_z, t) &= \langle\sigma''_z, t|\sigma'_z, 0\rangle = \sum_{\sigma'''_{z'}}\langle\sigma''_z, t|\sigma'''_{z'}, t\rangle\langle\sigma'''_{z'}, t|\sigma'_z, 0\rangle \\ &= \sum_{\sigma'''_{z'}}\psi_{\sigma'''_{z'}}(\sigma''_z, 0)\langle\sigma'''_{z'}, t|\sigma'_z, 0\rangle,\end{aligned} \tag{10.69}$$

where we have noted that

$$\langle\sigma''_z, t|\sigma'''_{z'}, t\rangle = \langle\sigma''_z, 0|\sigma'''_{z'}, 0\rangle. \tag{10.70}$$

The last transformation function in Eq. (10.69) has a simple time dependence, since it satisfies

$$i\hbar\frac{\partial}{\partial t}\langle\sigma'''_{z'}, t|\sigma'_z, 0\rangle = -\hbar\omega\langle\sigma'''_{z'}, t|\sigma_{z'}|\sigma'_z, 0\rangle = -\hbar\omega\sigma'''_{z'}\langle\sigma'''_{a'}, t|\sigma'_z, 0\rangle, \tag{10.71}$$

which integrates to

$$\langle \sigma'''_{a'}, t|\sigma'_z, 0\rangle = e^{i\omega\sigma'''_{z'} t}\langle \sigma'''_{a'}, 0|\sigma'_z, 0\rangle = \alpha_{\sigma'''_{z'}}(t). \tag{10.72}$$

Thus, for example,

$$\begin{aligned} \psi_{+z}(t) &= \psi_{+z'} e^{i\omega t}\langle +z'| + z\rangle + \psi_{-z'} e^{-i\omega t}\langle -z'| + z\rangle \\ &= \psi_{+z'} e^{i\omega t}\psi_{+z'}(+)^* + \psi_{-z'} e^{-i\omega t}\psi_{-z'}(+)^* \\ &= \cos\frac{\theta}{2} e^{i\phi/2} e^{i\omega t}\psi_{+z'} - \sin\frac{\theta}{2} e^{i\phi/2} e^{-i\omega t}\psi_{-z'}, \end{aligned} \tag{10.73}$$

which coincides with Eq. (10.68).

Our original question was to compute the probability of the spin remaining in its original orientation. For example, what is $p(+z, t; +z, 0)$? The corresponding amplitude is

$$\begin{aligned} \langle +z, t| + z, 0\rangle &= \psi_{+z}(+, t) \\ &= \cos\frac{\theta}{2} e^{i\phi/2} e^{i\omega t}\psi_{+z'}(+) - \sin\frac{\theta}{2} e^{i\phi/2} e^{-i\omega t}\psi_{-z'}(+) \\ &= \cos^2\frac{\theta}{2} e^{i\omega t} + \sin^2\frac{\theta}{2} e^{-i\omega t}, \end{aligned} \tag{10.74}$$

where the last, evidently, reduces to 1 at $t = 0$. Therefore the probability is

$$\begin{aligned} p(+z, t; +z, 0) &= |\psi_{+z}(+, t)|^2 \\ &= \cos^4\frac{\theta}{2} + \sin^4\frac{\theta}{2} + 2\cos^2\frac{\theta}{2}\sin^2\frac{\theta}{2}\cos 2\omega t \\ &= 1 - 4\cos^2\frac{\theta}{2}\sin^2\frac{\theta}{2}\frac{1 - \cos 2\omega t}{2} \\ &= 1 - \sin^2\theta\sin^2\omega t. \end{aligned} \tag{10.75}$$

We check this by computing the probability for the spin to flip:

$$\begin{aligned} p(-z, t; +z, 0) &= |\psi_{+z}(-, t)|^2 \\ &= |\cos\frac{\theta}{2}\sin\frac{\theta}{2} e^{i\phi} e^{i\omega t} - \cos\frac{\theta}{2}\sin\frac{\theta}{2} e^{i\phi} e^{-i\omega t}|^2 \\ &= \cos^2\frac{\theta}{2}\sin^2\frac{\theta}{2}(2 - 2\cos 2\omega t) = \sin^2\theta\sin^2\omega t, \end{aligned} \tag{10.76}$$

which agrees with Eq. (10.75).