Physics 221A
Fall 2005
Notes 16
Time Reversal

16.1. Introduction

We have now considered the space-time symmetries of translations, proper rotations, and spatial inversions (that is, improper rotations) and the operators that implement these symmetries on a quantum mechanical system. We now turn to the last of the space-time symmetries, namely, time reversal. As we shall see, time reversal is different from all the others, in that it is implemented by means of antiunitary transformations.

16.2. Time Reversal in Classical Mechanics

Consider the classical motion of a single particle in three-dimensional space. Its trajectory $\mathbf{r}(t)$ is a solution of the equations of motion, $\mathbf{F} = m\mathbf{a}$. We define the time-reversed classical motion as $\mathbf{r}(-t)$. It is the motion we would see if we took a movie of the original motion and ran it backwards. Is the time-reversed motion also physically allowed (that is, does it also satisfy the classical equations of motion)?

The answer depends on the nature of the forces. Consider, for example, the motion of a charged particle of charge q in an electric field $\mathbf{E} = -\nabla\phi$, for which the equations of motion are

$$m\frac{d^2\mathbf{r}}{dt^2} = q\mathbf{E}(\mathbf{r}). \tag{16.1}$$

If $\mathbf{r}(t)$ is a solution of these equations, then so is $\mathbf{r}(-t)$, as follows easily from the fact that the equations are second order in time, so that the two changes of sign coming from $t \to -t$ cancel. However, this property does not hold for magnetic forces, for which the equations of motion include first order time derivatives:

$$m\frac{d^2\mathbf{r}}{dt^2} = \frac{q}{c}\frac{d\mathbf{r}}{dt}\times\mathbf{B}(\mathbf{r}). \tag{16.2}$$

In this equation, the left-hand side is invariant under $t \to -t$, while the right-hand side changes sign. For example, in a constant magnetic field, the sense of the circular motion of a charged particle (clockwise or counterclockwise) is determined by the charge of the particle, not the initial conditions, and the time-reversed motion $\mathbf{r}(-t)$ has the wrong sense.

We see that motion in a given electric field is time-reversal invariant, while in a magnetic field it is not.

We must add, however, that whether a system is time-reversal invariant depends on the definition of "the system." In the examples above, we were thinking of the system as consisting of a single charged particle, moving in given fields. But if we enlarge "the system" to include the charges that produce the fields (electric and magnetic), then we will find that time-reversal invariance is restored, even in the presence of magnetic fields. This is because when we set $t \to -t$, the velocities of all the particles change sign, so the current does also. But this change does nothing to the charges of the particles, so the charge density is left invariant. Thus, the rules for transforming charges and currents under time reversal is

$$\rho \to \rho, \qquad \mathbf{J} \to -\mathbf{J}. \tag{16.3}$$

But according to Maxwell's equations, this implies the transformation laws

$$\mathbf{E} \to \mathbf{E}, \qquad \mathbf{B} \to -\mathbf{B}, \tag{16.4}$$

for the electromagnetic field under time reversal. With these rules, we see that time-reversal invariance is restored to Eq. (16.2), since there are now two changes of sign on the right hand side.

Thus we have worked out the basic transformation properties of the electromagnetic field under time reversal, and we find that electromagnetic effects are overall time-reversal invariant. We have shown this only at the classical level, but in fact it is true at the quantum level as well.

Similarly, in quantum physics we are often interested in the time-reversal invariance of a given system, such as an atom interacting with external fields. The usual point of view is to take the external fields as just given, and not to count them as part of the system. Under these circumstances the atomic system is time-reversal invariant if there are no external magnetic fields, but time-reversal invariance is broken in their presence. On the other hand, the atom generates its own, internal, magnetic fields, such as the dipole fields associated with the magnetic moments of electrons or nuclei, or the magnetic field produced by the moving charges. Since, however, these fields are produced by charges that are a part of "the system," they do not break time-reversal invariance.

16.3. Time Reversal and the Schrödinger Equation

Let us now consider the quantum analog of Eq. (16.1), that is, the motion of a charged particle in a given electric field. The Schrödinger equation in this case is

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \Bigl[-\frac{\hbar^2}{2m}\nabla^2 + q\phi(\mathbf{r})\Bigr]\psi(\mathbf{r},t). \tag{16.5}$$

As we can easily see, if $\psi(\mathbf{r},t)$ is a solution to this version of the time-dependent Schrödinger equation, then $\psi^*(\mathbf{r},-t)$ is also, and we take the latter as the time-reversed solution. It is necessary to take the complex conjugate, because without it, the left-hand side of Eq. (16.5) would change sign under $t \to -t$. We can see already from this example that time reversal in quantum mechanics is represented by an antilinear operator, since a linear operator is unable to map a wave function into its complex conjugate.

Similarly, the quantum analog of Eq. (16.2) is the Schrödinger equation for a particle in a magnetic field,

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \frac{1}{2m}\Bigl[-i\hbar\nabla - \frac{q}{c}\mathbf{A}(\mathbf{r})\Bigr]^2\psi(\mathbf{r},t). \tag{16.6}$$

In this case if $\psi(\mathbf{r},t)$ is a solution, it does not follow that $\psi^*(\mathbf{r},-t)$ is also a solution, because of the terms that are linear in $\mathbf{A}$. But $\psi^*(\mathbf{r},-t)$ is a solution in the reversed magnetic field, that is, after the replacement $\mathbf{A} \to -\mathbf{A}$. This is just as in the classical case.

16.4. The Time-Reversal Operator Θ

In quantum mechanics we will be interested in a time-reversal operator, which we denote by Θ. This operator acts on kets of our quantum mechanical state space, and does not by itself involve the time. (The operator Θ is time-independent.) Rather, if we think of a ket $|\psi(0)\rangle$ as the initial condition for the time-dependent Schrödinger equation, then we will regard the ket $\Theta|\psi(0)\rangle$ as the initial condition for the time-reversed motion. As we will see, the time-reversed motion itself is given by

$$|\psi_r(t)\rangle = \Theta|\psi(-t)\rangle. \tag{16.7}$$

The time-reversal operator will be required to satisfy a set of postulates. First, since probabilities should be conserved under time reversal, we require

$$\Theta^\dagger\Theta = 1. \tag{16.8}$$

Next, in classical mechanics, the initial conditions of a motion $\mathbf{r}(t)$ transform under time reversal according to $(\mathbf{r}_0,\mathbf{p}_0) \to (\mathbf{r}_0,-\mathbf{p}_0)$, so we postulate that the time-reversal operator in quantum mechanics satisfies the conjugation relations,

$$\Theta\mathbf{r}\Theta^\dagger = \mathbf{r}, \qquad \Theta\mathbf{p}\Theta^\dagger = -\mathbf{p}, \tag{16.9}$$

from which follows

$$\Theta \mathbf{L} \Theta^\dagger = -\mathbf{L}. \tag{16.10}$$

We will generalize this latter equation and suppose that it applies to all kinds of angular momentum, orbital as well as spin, so that

$$\Theta \mathbf{J} \Theta^\dagger = -\mathbf{J}. \tag{16.11}$$

This is reasonable, for if we think of a simple model of a charged spinning particle as a charged, rotating sphere, then we see that reversing the motion will reverse both the angular momentum as well as the magnetic field produced by the spin. We take Eqs. (16.8), (16.9) and (16.11) as the postulates that Θ must satisfy.

16.5. Θ Cannot Be Unitary

It turns out that the conjugation relations (16.9) cannot be satisfied by any unitary operator. For if we take the canonical commutation relations,

$$[r_i, p_j] = i\hbar\, \delta_{ij}, \tag{16.12}$$

and conjugate with Θ, we find

$$\Theta [r_i, p_j] \Theta^\dagger = -[r_i, p_j] = -i\hbar\, \delta_{ij} = \Theta (i\hbar\, \delta_{ij}) \Theta^\dagger. \tag{16.13}$$

This leads to a contradiction if Θ is a unitary operator, and we are forced to conclude that the time-reversal operator Θ must be antilinear, so that the imaginary unit i on the right-hand side of Eq. (16.13) will change into $-i$ when Θ is pulled through it.

16.6. Wigner's Theorem

There is a famous theorem, proved by Wigner, that says that if we have a mapping of a ket space onto itself, taking, say, kets $|\psi\rangle$ and $|\phi\rangle$ into kets $|\psi'\rangle$ and $|\phi'\rangle$, such that the absolute values of all scalar products are preserved, that is, such that

$$|\langle \psi | \phi \rangle| = |\langle \psi' | \phi' \rangle| \tag{16.14}$$

for all $|\psi\rangle$ and $|\phi\rangle$, then, to within inessential phase factors, the mapping must be either a linear unitary operator or an antilinear unitary operator. The reason Wigner does not demand that the scalar products themselves be preserved (only their absolute values) is that the only quantities that are physically measurable are absolute squares of scalar products. These are the probabilities that are experimentally measurable. This theorem is discussed in more detail by Messiah, *Quantum Mechanics*, in which a proof is given. (See also Steven Weinberg, *The Quantum Theory of Fields I.*) Its relevance for the discussion of symmetries in quantum mechanics is that a symmetry operation must preserve the probabilities of all experimental outcomes, and thus all symmetries must be implemented either by unitary or antiunitary operators. In fact, all symmetries except time reversal (translations, proper rotations, parity, and others as well) are implemented by unitary operators. Time reversal, however, requires antiunitary operators.

16.7. Properties of Antilinear Operators

Since we have not encountered antilinear operators before, we now make a digression to discuss their mathematical properties. We let $\mathcal{E}$ be the ket space of some quantum mechanical system. In the following general discussion we denote linear operators by L, L_1, etc., and antilinear operators by A, A_1, etc. Both linear and antilinear operators are mappings of the ket space onto itself,

$$\begin{aligned} L &: \mathcal{E} \to \mathcal{E}, \\ A &: \mathcal{E} \to \mathcal{E}, \end{aligned} \tag{16.15}$$

but they have different distributive properties when acting on linear combinations of kets:

$$L\big(c_1|\psi_1\rangle + c_2|\psi_2\rangle\big) = c_1\, L|\psi_1\rangle + c_2\, L|\psi_2\rangle \tag{16.16a}$$

$$A\big(c_1|\psi_1\rangle + c_2|\psi_2\rangle\big) = c_1^*\, A|\psi_1\rangle + c_2^*\, A|\psi_2\rangle \tag{16.16b}$$

(see Eqs. (1.34)). In particular, an antilinear operator does not commute with a constant, when the latter is regarded as a multiplicative operator in its own right. Rather, we have

$$\boxed{Ac = c^* A.} \tag{16.17}$$

It follows from these definitions that the product of two antilinear operators is linear, and the product of a linear with an antilinear operator is antilinear. More generally, a product of operators is either linear or antilinear, depending on whether the number of antilinear factors is even or odd, respectively.

We now have to rethink the entire Dirac bra-ket formalism, to incorporate antilinear operators. To begin, we define the action of antilinear operators on bras. We recall that a bra, by definition, is a complex-valued, linear operator on kets, that is, a mapping,

$$\text{bra} : \mathcal{E} \to \mathbb{C}, \tag{16.18}$$

and that the value of a bra acting on a ket is just the usual scalar product. Thus, if $\langle\phi|$ is a bra, then we have

$$\big(\langle\phi|\big)\big(|\psi\rangle\big) = \langle\phi|\psi\rangle. \tag{16.19}$$

We now suppose that an antilinear operator A is given, that is, its action on kets is known, and we wish to define its action on bras. For example, if $\langle\phi|$ is a bra, we wish to define $\langle\phi|A$. In the case of linear operators, the definition was

$$\big(\langle\phi|L\big)\big(|\psi\rangle\big) = \big(\langle\phi|\big)\big(L|\psi\rangle\big). \tag{16.20}$$

Since the positioning of the parentheses is irrelevant, it is customary to drop them, and to write simply $\langle\phi|L|\psi\rangle$. In other words, we can think of L as acting either to the right or to the left. However, the analogous definition for antilinear operators does not work, for if we try to write

$$\big(\langle\phi|A\big)\big(|\psi\rangle\big) = \big(\langle\phi|\big)\big(A|\psi\rangle\big), \tag{16.21}$$

then $\langle\phi|A$ is indeed a complex-valued operator acting on kets, but it is an antilinear operator, not a linear one. Bras are supposed to be linear operators. Therefore we introduce a complex conjugation to make $\langle\phi|A$ a linear operator on kets, that is, we set

$$\boxed{\big(\langle\phi|A\big)|\psi\rangle = \big[\langle\phi|\big(A|\psi\rangle\big)\big]^*.} \tag{16.22}$$

This rule is easiest to remember in words: we say that in the case of an antilinear operator, it *does* matter whether the operator acts to the right or to the left in a matrix element, and if we change the direction in which the operator acts, we must complex conjugate the matrix element. In the case of antilinear operators, parentheses are necessary to indicate which direction the operator acts. The parentheses are awkward, and the fact is that Dirac's bra-ket notation is not as convenient for antilinear operators as it is for linear ones.

Next we consider the definition of the Hermitian conjugate. We recall that in the case of linear operators, the Hermitian conjugate is defined by

$$L^\dagger|\psi\rangle = \big(\langle\psi|L\big)^\dagger, \tag{16.23}$$

for all kets $|\psi\rangle$, or equivalently by

$$\langle\phi|L^\dagger|\psi\rangle = \langle\psi|L|\phi\rangle^*, \tag{16.24}$$

for all kets $|\psi\rangle$ and $|\phi\rangle$. Here the linear operator L is assumed given, and we are defining the new linear operator $L^\dagger$. The definition (16.23) also works for antilinear operators, that is, we set

$$A^\dagger|\psi\rangle = \big(\langle\psi|A\big)^\dagger. \tag{16.25}$$

We note that by this definition, $A^\dagger$ is an antilinear operator if A is antilinear. Now, however, when we try to write the analog of (16.24), we must be careful about the parentheses. Thus, we have

$$\langle\phi|\bigl(A^\dagger|\psi\rangle\bigr) = \bigl[\bigl(\langle\psi|A\bigr)|\phi\rangle\bigr]^*, \tag{16.26}$$

or, in view of Eq. (16.22),

$$\boxed{\langle\phi|\bigl(A^\dagger|\psi\rangle\bigr) = \langle\psi|\bigl(A|\phi\rangle\bigr).} \tag{16.27}$$

The boxed equations (16.17), (16.22) and (16.27) summarize the principal rules for antilinear operators that differ from those of linear operators.

16.8. Antiunitary Operators

We wrote down Eq. (16.8) thinking that it would require probabilities to be preserved under Θ. This would certainly be true if Θ were unitary, but since we now know Θ must be antilinear, we should think about probability conservation under antilinear transformations.

We define an *antiunitary* operator A as an antilinear operator that satisfies

$$AA^\dagger = A^\dagger A = 1. \tag{16.28}$$

We note that the product $AA^\dagger$ or $A^\dagger A$ is a linear operator. Just like unitary operators, antiunitary operators preserve the absolute values of scalar products, as indicated by Wigner's theorem. To see this, we let $|\psi\rangle$ and $|\phi\rangle$ be arbitrary kets, and we set $|\psi'\rangle = A|\psi\rangle$, $|\phi'\rangle = A|\phi\rangle$, where A is antiunitary. Then we have

$$\langle\phi'|\psi'\rangle = \bigl(\langle\phi|A^\dagger\bigr)\bigl(A|\psi\rangle\bigr) = \bigl[\langle\phi|\bigl(A^\dagger A|\psi\rangle\bigr)\bigr]^* = \langle\phi|\psi\rangle^*, \tag{16.29}$$

where we use Eq. (16.22) in the second equality and Eq. (16.28) in the third. Antiunitary operators take scalar products into their complex conjugates, and Eq. (16.14) is satisfied. Thus, we were correct in writing down Eq. (16.8) for probability conservation under time reversal.

16.9. The LK Decomposition

Given an antilinear operator A of interest, it is often convenient to factor it into the form

$$A = LK, \tag{16.30}$$

where L is a linear operator and K is a particular antilinear operator chosen for its simplicity. The idea is that K takes care of the antilinearity of A, while L takes care of all the rest. The choices made for K are usually of the following type.

Let Q stand for a complete set of commuting observables (a single symbol Q for all operators in the set). Let n be the collective set of quantum numbers corresponding to Q, so that the basis kets in this representation are $|n\rangle$. The index n can include continuous quantum numbers as well as discrete ones. Then we define a particular antilinear operator K_Q by requiring, first, that K_Q be antilinear, and second, that

$$K_Q|n\rangle = |n\rangle. \tag{16.31}$$

Notice that the definition of K_Q depends not only on the operators Q that make up the representation, but also the phase conventions for the eigenkets $|n\rangle$. If K_Q were a linear operator, Eq. (16.31) would imply $K_Q = 1$; but since K_Q is antilinear, the equation $K_Q = 1$ is not only not true, it is meaningless, since it equates an antilinear operator to a linear one. But Eq. (16.31) does completely specify K_Q, for if $|\psi\rangle$ is an arbitrary ket, expanded according to

$$|\psi\rangle = \sum_n c_n|n\rangle, \tag{16.32}$$

then

$$K_Q|\psi\rangle = \sum_n c_n^*|n\rangle, \tag{16.33}$$

where we use Eqs. (16.16b) and (16.31). Thus, the action of K_Q on an arbitrary ket is known. The effect of K_Q is to bring about a complex conjugation of the expansion coefficients in the Q representation. These expansion coefficients are the same as the wavefunction in the Q representation; thus, in wave function language in the Q representation, K_Q just maps the wave function into its complex conjugate.

Consider, for example, the ket space for a spinless particle in three dimensions. Here we can work in the position representation, in which $Q = \mathbf{r}$ and in which the basis kets are $|\mathbf{r}_0\rangle$ (we write $\mathbf{r}$ for the operators, and $\mathbf{r}_0$ for the eigenvalues). Then we define the antilinear operator $K_\mathbf{r}$ by

$$K_\mathbf{r}|\mathbf{r}_0\rangle = |\mathbf{r}_0\rangle, \tag{16.34}$$

so that if $|\psi\rangle$ is an arbitrary ket and $\psi(\mathbf{r}_0)$ its wavefunction, then

$$K_\mathbf{r}|\psi\rangle = K_\mathbf{r}\int d^3\mathbf{r}_0\,|\mathbf{r}_0\rangle\langle\mathbf{r}_0|\psi\rangle = K_\mathbf{r}\int d^3\mathbf{r}_0\,\psi(\mathbf{r}_0)|\mathbf{r}_0\rangle = \int d^3\mathbf{r}_0\,\psi^*(\mathbf{r}_0)|\mathbf{r}_0\rangle. \tag{16.35}$$

Thus, $\psi(\mathbf{r}_0)$ is mapped into $\psi(\mathbf{r}_0)^*$.

The operator K_Q looks simple in the Q-representation. It may of course be expressed in other representations, but then it no longer looks so simple. For example, $K_{\mathbf{r}}$ is not as simple in the momentum representation as in the configuration representation (an explicit expression for $K_{\mathbf{r}}$ in the momentum representation will be left as an exercise).

It follows from the definition (16.31) that K_Q satisfies

$$K_Q^2 = 1. \tag{16.36}$$

(Just multiply Eq. (16.31) by K_Q and note that K_Q^2 is a linear operator, so that Eq. (16.36) is meaningful.) The operator K_Q also satisfies

$$K_Q = K_Q^\dagger, \tag{16.37}$$

and is therefore antiunitary. To prove this, we write

$$\begin{aligned} K_Q^\dagger|n\rangle &= \sum_m |m\rangle\langle m|\big(K_Q^\dagger|n\rangle\big) = \sum_m |m\rangle\langle n|\big(K_Q|m\rangle\big) \\ &= \sum_m |m\rangle\langle n|m\rangle = \sum_m |m\rangle\delta_{mn} = |n\rangle, \end{aligned} \tag{16.38}$$

where we use Eq. (16.27) in the second equality and (16.31) in the third. Since $K_Q^\dagger$ has the same effect on the basis kets as K, and since both are antilinear, they must be equal antilinear operators.

16.10. The Time-Reversed Motion

Suppose we have a Hamiltonian that commutes with time reversal,

$$[\Theta, H] = 0 \quad \text{or} \quad \Theta H \Theta^\dagger = H. \tag{16.39}$$

We have not defined Θ yet, but we will assume that some Θ exists that satisfies the postulates (16.8), (16.9) and (16.11). The time-dependent Schödinger equation is

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle. \tag{16.40}$$

If $|\psi(t)\rangle$ is a solution of this equation, then the time-reversed ket $|\psi_r(t)\rangle = \Theta|\psi(-t)\rangle$ is also a solution. To see this, we let $\tau = -t$, and follow the calculation,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi_r(t)\rangle &= i\hbar\frac{\partial}{\partial t}\Theta|\psi(-t)\rangle = -i\hbar\Theta\frac{\partial}{\partial \tau}|\psi(\tau)\rangle = \Theta i\hbar\frac{\partial}{\partial \tau}|\psi(\tau)\rangle \\ &= \Theta H|\psi(\tau)\rangle = H\Theta|\psi(\tau)\rangle = H|\psi_r(t)\rangle. \end{aligned} \tag{16.41}$$

Another approach to the same result is to write a solution of the Schrödinger equation as

$$|\psi(t)\rangle = \exp(-itH/\hbar)|\psi(0)\rangle, \tag{16.42}$$

to which we apply Θ,

$$\Theta|\psi(t)\rangle = \Theta\exp(-itH/\hbar)\Theta^\dagger\Theta|\psi(0)\rangle. \tag{16.43}$$

The conjugated time-evolution operator can be written,

$$\Theta\exp(-itH/\hbar)\Theta^\dagger = \exp\Big[\Theta(-itH/\hbar)\Theta^\dagger\Big] = \exp(+itH/\hbar), \tag{16.44}$$

where we have used the antilinearity of Θ and Eq. (16.39). Then by using Eq. (16.7) and replacing t by $-t$, Eq. (16.43) becomes

$$|\psi_r(t)\rangle = \exp(-itH/\hbar)|\psi_r(0)\rangle. \tag{16.45}$$

Thus, $|\psi_r(t)\rangle$ is also a solution of the time-dependent Schrödinger equation.

16.11. Examples of Hamiltonians

To see some examples of Hamiltonians that are invariant under time-reversal, we assume the validity of the commutation relations (16.9) and (16.11). Then a simple kinetic-plus-potential Hamiltonian in three dimensions,

$$H = \frac{|\mathbf{p}|^2}{2m} + V(\mathbf{r}), \tag{16.46}$$

certainly commutes with time reversal, because the kinetic energy is even in the momentum. We emphasize that the potential in Eq. (16.46) need not be a central force potential. More generally, a kinetic-plus-potential Hamiltonian for any number of particles in any number of dimensions commutes with time reversal.

The easiest way to break time-reversal invariance is to introduce a external magnetic field. Then the kinetic energy becomes

$$\frac{1}{2m}\Big[\mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{r})\Big]^2, \tag{16.47}$$

which does not commute with Θ because $\mathbf{p}$ changes sign under conjugation by Θ, while $\mathbf{A}(\mathbf{r})$ does not.

As mentioned previously, however, if the magnetic field is internally generated, then time-reversal invariance is not broken. For example, in an atom the spin-orbit interaction is the magnetic interaction between the spin of the electron and the magnetic field produced by the motion of the nucleus around the electron, as seen in the electron rest frame. It is described by a term in the Hamiltonian of the form

$$f(r)\mathbf{L}\cdot\mathbf{S}, \tag{16.48}$$

which according to Eq. (16.11) is invariant under time reversal (both $\mathbf{L}$ and $\mathbf{S}$ change sign). Similarly, spin-spin interactions such as hyperfine effects in an atom, which are proportional to $\mathbf{I}\cdot\mathbf{S}$ ($\mathbf{I}$ is the nuclear spin, $\mathbf{S}$ the electron spin) are invariant under time reversal.

Are there any examples of interactions that break time-reversal invariance but that only involve internally generated fields? Yes, suppose for example that the nucleus has an electric dipole moment, call it $\boldsymbol{\mu}_e$. By the Wigner-Eckart theorem, this vector is proportional to the spin $\mathbf{S}$, so we get a term in the Hamiltonian,

$$H_{\rm int} = -\boldsymbol{\mu}_e\cdot\mathbf{E} = k\mathbf{S}\cdot\mathbf{E}, \tag{16.49}$$

where k is a constant. This term is odd under time reversal, and so breaks time-reversal invariance. Time-reversal invariance is known to be respected to a very high degree of approximation, so terms of the form (16.49), if they are present in ordinary atoms, are very small.

16.12. Time Reversal in Spinless Systems

So far we have not stated what the time-reversal operator Θ actually is, only the properties we expect of it. The actual form of the time-reversal operator depends on the system under consideration. In the following we will work our way up from simple systems to more complicated ones, and define the time-reversal operator at each step.

Our first system is that of a spinless particle moving in three dimensions, for which the ket space is $\mathcal{E} = {\rm span}\{|\mathbf{r}_0\rangle\}$, where we use $\mathbf{r}_0$ for the eigenvalues of the operator $\mathbf{r}$. This ket space is of course isomorphic to the space of wave functions $\psi(\mathbf{r})$. In this case it turns out that the time-reversal operator Θ may be defined by

$$\Theta = K_{\mathbf{r}}, \tag{16.50}$$

where $K_{\mathbf{r}}$ is the complex conjugation operator in the $\mathbf{r}$-representation. To show this, we must check the conjugation relations (16.9). Consider first the operator $K\mathbf{r}K^\dagger$, where we write simply K for $K_{\mathbf{r}}$. We allow this to act on a basis ket, finding,

$$K\mathbf{r}K^\dagger|\mathbf{r}_0\rangle = K\mathbf{r}_0|\mathbf{r}_0\rangle = \mathbf{r}_0K|\mathbf{r}_0\rangle = \mathbf{r}_0|\mathbf{r}_0\rangle = \mathbf{r}|\mathbf{r}_0\rangle, \tag{16.51}$$

where we use $K|\mathbf{r}_0\rangle = |\mathbf{r}_0\rangle$ and remember that $K^\dagger = K$. Since this is true for arbitrary $|\mathbf{r}_0\rangle$, we have

$$K\mathbf{r}K^\dagger = \mathbf{r}. \tag{16.52}$$

Similarly, for the momentum operator we have

$$\begin{aligned} K\mathbf{p}K^\dagger|\mathbf{r}_0\rangle = K\mathbf{p}|\mathbf{r}_0\rangle = Ki\hbar\frac{\partial}{\partial\mathbf{r}_0}|\mathbf{r}_0\rangle = -i\hbar\frac{\partial}{\partial\mathbf{r}_0}K|\mathbf{r}_0\rangle \\ = -i\hbar\frac{\partial}{\partial\mathbf{r}_0}|\mathbf{r}_0\rangle = -\mathbf{p}|\mathbf{r}_0\rangle, \end{aligned} \tag{16.53}$$

or

$$K\mathbf{p}K^\dagger = -\mathbf{p}. \tag{16.54}$$

The definition (16.50) satisfies the commutation relations (16.9), and hence (16.11) (since $\mathbf{J} = \mathbf{L}$ for such systems).

This result can be easily generalized to the case of any number of spinless particles in any number of dimensions. The time-reversal operator Θ is defined as the complex conjugation operation in the configuration representation, so that its action on wave functions is given by

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_n) \xrightarrow{\Theta} \psi^*(\mathbf{r}_1, \ldots, \mathbf{r}_n). \tag{16.55}$$

This is a simple result that covers many cases occurring in practice.

16.13. Time Reversal and Energy Eigenfunctions

Let $|\psi\rangle$ be an energy eigenstate in a system that is time-reversal invariant,

$$H|\psi\rangle = E|\psi\rangle, \tag{16.56}$$

with $[H, \Theta] = 0$. Then we easily find

$$H(\Theta|\psi\rangle) = E(\Theta|\psi\rangle), \tag{16.57}$$

that is, Θ maps eigenstates of H into eigenstates of H with the same energy. If the original eigenstate is nondegenerate, then $\Theta|\psi\rangle$ must be proportional to $|\psi\rangle$,

$$\Theta|\psi\rangle = c|\psi\rangle, \tag{16.58}$$

where c is a constant. In fact, the constant is a phase factor, as we see by squaring both sides,

$$(\langle\psi|\Theta^\dagger)(\Theta|\psi\rangle) = [\langle\psi|(\Theta^\dagger\Theta|\psi\rangle)]^* = \langle\psi|\psi\rangle^* = 1 = |c|^2, \tag{16.59}$$

where we use Eqs. (16.8) and (16.22). Thus we can write

$$\Theta|\psi\rangle = e^{i\alpha}|\psi\rangle. \tag{16.60}$$

16.14. Reality of Wave Functions in Spinless Systems

In particular, for a spinless system in three dimensions with a kinetic-plus-potential Hamiltonian, Eq. (16.60) implies that nondegenerate energy eigenfunctions $\psi(\mathbf{r})$ satisfy,

$$\psi^*(\mathbf{r}) = e^{i\alpha}\,\psi(\mathbf{r}). \tag{16.61}$$

Now define a new wave function,

$$\phi(\mathbf{r}) = e^{i\alpha/2}\,\psi(\mathbf{r}), \tag{16.62}$$

so that

$$\phi(\mathbf{r}) = \phi^*(\mathbf{r}). \tag{16.63}$$

We see that a nondegenerate energy eigenfunction in a spinless kinetic-plus-potential system is always proportional to a real eigenfunction; the eigenfunction may be chosen to be real. (We invoked the identical argument earlier in the semester, when we showed that nondegenerate energy eigenfunctions in simple one-dimensional problems can always be chosen to be real.)

In the case of degeneracies, the eigenfunctions are not necessarily proportional to real eigenfunctions, but real eigenfunctions can always be constructed out of linear combinations of the degenerate eigenfunctions. We state this fact without proof, but we offer some examples. First, a free particle in one dimension has the degenerate energy eigenfunctions, $e^{ipx/\hbar}$ and $e^{-ipx/\hbar}$, both of which are intrinsically complex; but real linear combinations are $\cos(px/\hbar)$ and $\sin(px/\hbar)$.

Similarly, a spinless particle moving in a central force field in three dimensions possesses the energy eigenfunctions,

$$\psi_{n\ell m}(\mathbf{r}) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi), \tag{16.64}$$

which are degenerate since by the Wigner-Eckart theorem the energy $E_{n\ell}$ is independent of the magnetic quantum number m. The radial wave functions $R_{n\ell}$ can be chosen to be real, as we suppose, but the $Y_{\ell m}$'s are complex. However, in view of Eq. (12.41), we have

$$\psi^*_{n\ell m}(\mathbf{r}) = (-1)^m \psi_{n\ell,-m}(\mathbf{r}), \tag{16.65}$$

or, in ket language,

$$\Theta|n\ell m\rangle = (-1)^m |n\ell, -m\rangle. \tag{16.66}$$

In this case, real wave functions can be constructed out of linear combinations of the states $|n\ell m\rangle$ and $|n\ell, -m\rangle$. Sometimes it is convenient to ignore the radial variables and think of the Hilbert space of functions on the unit sphere, as we did in Notes 12; then we treat Θ as the complex conjugation operator acting on such functions, and we have

$$\Theta|\ell m\rangle = (-1)^m |\ell, -m\rangle, \tag{16.67}$$

instead of Eq. (16.66). This is a ket version of Eq. (12.41).

16.15. Time Reversal and Spin

Next we consider the spin degrees of freedom of a particle of spin s. For simplicity we will at first ignore the spatial degrees of freedom, so the $(2s+1)$-dimensional ket space is $\mathcal{E} = \text{span}\{|sm\rangle, m = -s, \ldots, s\}$. As usual, the basis kets are eigenstates of S_z. The postulated time-reversal operator must satisfy the conjugation relations,

$$\Theta \mathbf{S} \Theta^\dagger = -\mathbf{S}. \tag{16.68}$$

As we will show, this condition determines Θ to within an phase factor.

First we consider the operator S_z, which satisfies

$$\Theta S_z \Theta^\dagger = -S_z. \tag{16.69}$$

From this it easily follows that the ket $\Theta|sm\rangle$ is an eigenket of S_z with eigenvalue $-m\hbar$,

$$S_z \Theta|sm\rangle = -\Theta S_z|sm\rangle = -m\hbar\Theta|sm\rangle. \tag{16.70}$$

But since the eigenkets of S_z are nondegenerate, we must have

$$\Theta|sm\rangle = c_m|s, -m\rangle, \tag{16.71}$$

where c_m is a constant that presumably depends on m. In fact, if we square both sides of Eq. (16.71) and use the fact that Θ is antiunitary, we will see that c_m is a phase factor. To find the m-dependence of c_m, we study the commutation relations of Θ with the raising and lowering operators. For example, for S_+, we have

$$\Theta S_+ \Theta^\dagger = \Theta(S_x + iS_y)\Theta^\dagger = -S_x + iS_y = -S_-, \tag{16.72}$$

where we use Eq. (16.11) and where a second sign reversal takes place in the S_y-term due to the imaginary unit i. There is a similar equation for S_-; we summarize them both by writing

$$\Theta S_\pm \Theta^\dagger = -S_\mp. \tag{16.73}$$

Now let us apply S_+ to the ket $\Theta|sm\rangle$, and use the commutation relations (16.72). We find

$$\begin{aligned} S_+\Theta|sm\rangle &= -\Theta S_-|sm\rangle = -\hbar\sqrt{(s+m)(s-m+1)}\,\Theta|s,m-1\rangle \\ &= -\hbar\sqrt{(s+m)(s-m+1)}\,c_{m-1}\,|s,-m+1\rangle = c_m S_+|s,-m\rangle \\ &= \hbar\sqrt{(s+m)(s-m+1)}\,c_m|s,-m+1\rangle. \end{aligned} \tag{16.74}$$

But this implies

$$c_{m-1} = -c_m, \tag{16.75}$$

so c_m changes by a sign every time m increments or decrements by 1. Thus we have

$$c_m = c_{-s}\,(-1)^{m+s} = c_{-s}\,i^{2m+2s}. \tag{16.76}$$

We shall prefer the final form in this equation, since s and m may be half integers, and we prefer to work with integer exponents.

To summarize, it is a direct consequence of the conjugation relation (16.68) that the action of the time-reversal operator on the basis kets is given by

$$\Theta|sm\rangle = \eta\,i^{2m}|s,-m\rangle, \tag{16.77}$$

where we set $\eta = c_{-s}i^{2s}$. This proves our earlier assertion, that Θ is determined to within a phase by the conjugation relation (16.68).

Since the phase η is independent of m, it can be absorbed into the definition of Θ, by writing, say, $\Theta = \eta\Theta_1$, where Θ_1 is a new time-reversal operator. Such an overall phase has no effect on the desired commutation relations (16.11), as one can easily verify, and in fact is devoid of physical significance. One choice for η that is commonly in use is to take $\eta = 1$, in which case we have simply

$$\Theta|sm\rangle = i^{2m}|s,-m\rangle. \tag{16.78}$$

This phase convention is nice because it is the obvious generalization of Eq. (16.66), which applies to orbital angular momentum.

16.16. Another Approach to Time Reversal and Spin

Another approach to finding a time-reversal operator that satisfies Eq. (16.68) is to attempt an LK-decomposition of Θ. Since the usual basis is the S_z basis, we examine the antiunitary operator K_{S_z}, for which we simply write K in the following. We begin by conjugating $\mathbf{S}$ by K, finding,

$$K \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} K^\dagger = \begin{pmatrix} S_x \\ -S_y \\ S_z \end{pmatrix}. \tag{16.79}$$

The operators S_x and S_z did not change sign because their matrices in the standard angular momentum basis are real (see Sec. 11.9), while S_y does change sign since its matrix for S_y is purely imaginary. We see that Θ is not equal to K, because the latter only changes the sign of one of the components of spin.

Nevertheless, the result can be fixed up with a unitary operator. Let U_0 be the spin rotation by angle π about the y-axis,

$$U_0 = U(\hat{\mathbf{y}}, \pi) = e^{-i\pi S_y/\hbar}. \tag{16.80}$$

Such a rotation leaves the y-component of a vector invariant, while flipping the signs of the x- and z-components. This is really an application of the adjoint formula (11.57). Thus we have

$$U_0 \begin{pmatrix} S_x \\ -S_y \\ S_z \end{pmatrix} U_0^\dagger = \begin{pmatrix} -S_x \\ -S_y \\ -S_z \end{pmatrix}. \tag{16.81}$$

Altogether, we can satisfy the requirement (16.68) by defining

$$\Theta = e^{-i\pi S_y/\hbar} K = K e^{-i\pi S_y/\hbar}, \tag{16.82}$$

where $e^{-i\pi S_y/\hbar}$ and K commute because the matrix for $e^{-i\pi S_y/\hbar}$ in the standard basis is real.

Comparing the approach of this section to that in Sec. 16.15), the operator Θ defined by Eq. (16.82) must be the same as that defined in Eq. (16.77), for some choice of η. In fact, with some additional trouble one can show that $\eta = i^{-2s}$ works (although this is not a very important fact, since η is nonphysical anyway).

16.17. Spatial and Spin Degrees of Freedom

Let us now include the spatial degress of freedom, and consider the case of a spinning particle in three-dimensional space. The ket space is $\mathcal{E} = \text{span}\{|\mathbf{r}, m\rangle\}$, following the notation of Eq. (14.10), and the wave functions are $\psi_m(\mathbf{r})$, as in Eq. (14.12). In this case, the obvious definition of the time-reversal operator is the product of the two operators introduced above ($\Theta = K_{\mathbf{r}}$ for the spatial degrees of freedom, and $\Theta = K_{S_z} U_0$ for the spin degrees of freedom). That is, we take

$$\Theta = Ke^{-i\pi S_y/\hbar}, \tag{16.83}$$

where now $K = K_{\mathbf{r}S_z}$ is the complex conjugation operator in the $|\mathbf{r}m\rangle$ basis, and where the rotation operator only rotates the spin (not the spatial degrees of freedom). This is the same as Eq. (16.82), except for a reinterpretation of the operator K.

For example, in the case of a spin-$\frac{1}{2}$ particle, we have $S_y = (\hbar/2)\sigma_y$, so

$$e^{-i\pi S_y/\hbar} = e^{-i(\pi/2)\sigma_y} = \cos(\pi/2) - i\sigma_y \sin(\pi/2) = -i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{16.84}$$

so a two component spinor as in Eq. (14.13) transforms under time reversal according to

$$\begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix} \xrightarrow{\Theta} \begin{pmatrix} -\psi_-^*(\mathbf{r}) \\ \psi_+^*(\mathbf{r}) \end{pmatrix}. \tag{16.85}$$

More generally, for any s the wave function $\psi_m(\mathbf{r})$ transforms under time-reversal according to

$$\psi_m(\mathbf{r}) \xrightarrow{\Theta} \sum_{m'} d^s_{mm'}(\pi)\, \psi^*_{m'}(\mathbf{r}), \tag{16.86}$$

where we use the reduced rotation matrices defined by Eq. (11.50). Compare this to Eq. (16.55) for a spinless particle.

Finally, to implement time reversal on a system of many spinning particles, for which the ket space is the tensor product of the ket spaces for the individual particles (both orbital and spin), we simply take Θ to be a product of operators of the form (16.83), one for each particle. The result is the formula (16.83) all over again, with K now interpreted as the complex conjugation in the tensor product basis,

$$|\mathbf{r}_{01} m_{s1}\rangle \otimes \ldots \otimes |\mathbf{r}_{0n} m_{sn}\rangle, \tag{16.87}$$

where n is the number of particles, and where the spin rotation is the product of the individual spin rotations,

$$e^{-i\pi S_y/\hbar} = e^{-i\pi S_{1y}/\hbar} \ldots e^{-i\pi S_{ny}/\hbar}. \tag{16.88}$$

Here S_y is the y-component of the total spin of the system,

$$S_y = S_{1y} + \ldots + S_{ny}. \tag{16.89}$$

It may seem strange that a rotation about the y-axis should appear in Eq. (16.82) or (16.83), since the time-reversal operator should not favor any particular direction in space.

Actually, the time-reversal operator does not favor any particular direction, it is just the decomposition into the indicated unitary operator $e^{-i\pi S_y/\hbar}$ and the antiunitary complex conjugation operator K which has treated the three directions in an asymmetrical manner. That is, the complex conjugation antiunitary operator K is tied to the S_z representation and the standard phase conventions used in angular momentum theory; since K does not treat the three directions symmetrically, the remaining unitary operator $e^{-i\pi S_y/\hbar}$ cannot either. However, their product does.

Often in multiparticle systems we will be interested to combine spin states of individual particles together to form eigenstates of total S^2 and S_z. This will give us a complete set of commuting observables that will include the total S^2 and S_z, rather than the S_z's of individual particles as in Eq. (16.87). But since the Clebsch-Gordan coefficients are real, the complex conjugation operator K in the new basis will be the same as in the old, and Eq. (16.83) will still hold.

16.18. Kramers Degeneracy

Equation (16.83) allows us to compute the square of Θ, which is used in an important theorem to be discussed momentarily. We find

$$\Theta^2 = Ke^{-i\pi S_y/\hbar}Ke^{-i\pi S_y/\hbar} = e^{-2\pi i S_y/\hbar}, \tag{16.90}$$

where we commute K past the rotation and use $K^2 = 1$. The result is a total spin rotation of angle 2π about the y-axis. This rotation can be factored into a product on spin rotations, one for each particle, as in Eq. (16.88). For every boson, that is, for every particle with integer spin, the rotation by 2π is $+1$, while for every fermion, that is, for every particle of half-integer spin, the rotation by 2π is -1, because of the double-valued representation of the classical rotations for the case of half-integer angular momentum. Thus, the product (16.90) is $+1$ if the system contains an even number of fermions, and -1 if it contains an odd number.

As an application of the time-reversal operator, consider an arbitrarily complex system of possibly many spinning particles, in which the Hamiltonian is invariant under time reversal. One may think, for example, of the electronic motion in a solid or a molecule. There is no assumption that the system be invariant under rotations; this would not usually be the case, for example, in the electronic motion in the molecule. Suppose such a system has a nondegenerate energy eigenstate $|\psi\rangle$ with eigenvalue E, as in Sec. 16.13, so that $|\psi\rangle$ satisfies Eq. (16.60). Now multiplying that equation by Θ, we obtain

$$\Theta^2|\psi\rangle = \Theta e^{i\alpha}|\psi\rangle = e^{-i\alpha}\Theta|\psi\rangle = |\psi\rangle. \tag{16.91}$$

But if the system contains an odd number of fermions, then according to Eq. (16.90) we must have $\Theta^2 = -1$, which contradicts Eq. (16.91). Therefore the assumption of a nondegenerate energy level must be incorrect. We conclude that in time-reversal invariant systems with an odd number of fermions, the energy levels are always degenerate. This is called *Kramers degeneracy*. More generally, one can show that in such systems, the energy levels have a degeneracy that is even. Kramers degeneracy is lifted by any effect that breaks the time-reversal invariance, notably external magnetic fields.