Physics 581Quantum Mechanics IIP. M. Goldbart, 3135 ESBHandout 17webusers.physics.illinois.edu/~goldbartUniversity of Illinois20 April 2010HOMEWORK 12goldbart@illinois.edu

1) Motion reversal in classical and quantum mechanics: In classical mechanics in its Hamiltonian form, the state of a particle moving in three dimensions can be specified by the canonically conjugate pair of coordinates and momentum vectors (\mathbf{q}, \mathbf{p}) . Consider the motion of the particle [i.e., the evolution in time t of the state, $(\mathbf{q}(t), \mathbf{p}(t))$] of an explicitly time-independent system that obeys the initial condition $(\mathbf{q}(t_0), \mathbf{p}(t_0)) = (\mathbf{q}_0, \mathbf{p}_0)$ at time t_0 , evolves until time $t_0 + t_1$, and is motion reversed at this time, so that

$$(\mathbf{q}(t_0+t_1),\mathbf{p}(t_0+t_1)) \to (\mathbf{q}'(t_0+t_1),\mathbf{p}'(t_0+t_1)) := (\mathbf{q}(t_0+t_1),-\mathbf{p}(t_0+t_1)).$$

This motion-reversed state then evolves until time $t_0 + 2t_1$, at which time the state has become $(\mathbf{q}'(t_0 + 2t_1), \mathbf{p}'(t_0 + 2t_1))$.

- a) We say that the system is motion-reversal invariant if, for all t_0 and t_1 , $(\mathbf{q}'(t_0 + 2t_1), \mathbf{p}'(t_0 + 2t_1)) = (\mathbf{q}_0, -\mathbf{p}_0)$. Explain briefly why this is a sensible definition of motion-reversal invariance.
- b) By translating the condition for motion reversal invariance from classical mechanics to quantum mechanics, show that the it becomes

$$\mathrm{e}^{-iHt_1/\hbar} \mathcal{T} \mathrm{e}^{-iHt_1/\hbar} |\psi\rangle = \mathcal{T} |\psi\rangle$$

for any state $|\psi\rangle$. Here, \mathcal{T} is the *motion-reversal operator*, which effects the transformation of any state $|\psi\rangle$ into the state $\mathcal{T}|\psi\rangle$ describing reversed motion.

c) Show that the condition found in part (b) can be reduced to:

$$\mathcal{T}(-iH)\mathcal{T}^{-1} = iH.$$

d) We shall explore some properties of antiunitary operators below; for now let us accept that the condition for motion-reversal invariance becomes

$$\mathcal{T}H \, \mathcal{T}^{-1} = \begin{cases} -H & \text{for } \mathcal{T} \text{ unitary;} \\ +H & \text{for } \mathcal{T} \text{ antiunitary} \end{cases}$$

Now, for a free particle the Hamiltonian H_0 is quadratic in the momentum and therefore motion-reversal invariant, i.e., $\mathcal{T}H_0\mathcal{T}^{-1} = H_0$, which requires the latter case: \mathcal{T} antiunitary; this property of \mathcal{T} continues to hold for particles that are not free. Establish the antiunitarity of the motion-reversal transformations used in Questions 2 and 3, viz.,

$$\begin{split} \Psi(\mathbf{r}) &\to & \Psi(\mathbf{r})^*, & \text{for a spinless particle;} \\ \Psi_{\alpha}(\mathbf{r}) &\to & \sum_{\beta=\pm 1/2} \sigma^y_{\alpha\beta} \Psi_{\beta}(\mathbf{r})^*, & \text{for a spin-half particle.} \end{split}$$

2) Motion-reversal for a spinless particle: Consider a single, spinless particle moving in the presence of a static potential $V(\mathbf{r})$. Its wave function evolves according to the timedependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t).$$

- a) Show that if $\Psi(\mathbf{r}, t)$ is a solution of the Schrödinger equation then so is the *motion-reversed* solution $\widetilde{\Psi}(\mathbf{r}, t) := \Psi(\mathbf{r}, -t)^*$. Identify the requisite properties of V for this result to hold. [Note that this is a *dynamical* result, hinging on whether or not the system (as described via its Hamiltonian) has motion-reversal-invariance symmetry.]
- b) To see that $\Psi(\mathbf{r}, t)$ does indeed describe the motion-reversed state, relative to $\Psi(\mathbf{r}, t)$, establish the following results and briefly discuss their significance:
 - (i) If $\Pi_t(\mathbf{r})$ is the probability of finding the particle at position \mathbf{r} at time t in the state $\Psi(\mathbf{r}, t)$ then in the motion-reversed state $\widetilde{\Psi}(\mathbf{r}, t)$ it is $\Pi_{-t}(\mathbf{r})$.
 - (ii) If $\Phi_t(\mathbf{p})$ is the probability of finding the particle to have momentum \mathbf{p} at time t in the state $\Psi(\mathbf{r}, t)$ then in the motion-reversed state $\widetilde{\Psi}(\mathbf{r}, t)$ it is $\Phi_{-t}(-\mathbf{p})$.
 - (iii) If $\langle \mathbf{L} \rangle_t$ is the expectation value of the orbital angular momentum of the particle in the state $\Psi(\mathbf{r}, t)$ then in the motion-reversed state $\widetilde{\Psi}(\mathbf{r}, t)$ it is $-\langle \mathbf{L} \rangle_{-t}$.

[Note that the properties established in part (b) are *kinematical* consequences of the motion-reversal transformation $\Psi(\mathbf{r}, t) \to \Psi(\mathbf{r}, -t)^*$. They hold regardless of whether or not the system (as described via its Hamiltonian) is motion-reversal invariant.]

- c) By analyzing the appropriate Hamiltonian, discuss whether or not motion-reversal invariance holds for a spinless charged particle that is subjected to
 - (i) a time-independent magnetic field;
 - (ii) a time-independent electric field;
 - (iii) a time-dependent electric field.

3) Motion-reversal for a spin-half particle: The state $|\Psi\rangle$ of a spin-half particle can be described via the spinor wave function $\Psi_{\alpha}(\mathbf{r})$, i.e., the amplitude $\langle \mathbf{r}, \alpha | \Psi \rangle$, where $|\mathbf{r}, \alpha \rangle$ is a simultaneous eigenket of the position and spin projection, \mathbf{R} and S_z , having respective eigenvalues \mathbf{r} and $\alpha\hbar$ (with $\alpha = \pm 1/2$). For such systems, the spinor wave function describing the motion-reversed state is obtained via the transformation

$$\Psi_{lpha}(\mathbf{r})
ightarrow \widetilde{\Psi}_{lpha}(\mathbf{r}) := \sum_{eta = \pm 1/2} \sigma^y_{lphaeta} \Psi_{eta}(\mathbf{r})^*,$$

where $(\sigma^y)_{\alpha\beta} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ is the *y* Pauli matrix.

To see that $\Psi_{\alpha}(\mathbf{r})$ does indeed describe the motion-reversed state, relative to $\Psi_{\alpha}(\mathbf{r})$, establish the following kinematical results and briefly discuss their significance:

- a) If $\Pi(\mathbf{r})$ is the probability of finding the particle at position \mathbf{r} in the state $\Psi_{\alpha}(\mathbf{r})$ then in the motion-reversed state $\widetilde{\Psi}_{\alpha}(\mathbf{r})$ it is $\Pi(\mathbf{r})$.
- b) If $\Phi(\mathbf{p})$ is the probability of finding the particle to have momentum \mathbf{p} in the state $\Psi_{\alpha}(\mathbf{r})$ then in the motion-reversed state $\tilde{\Psi}_{\alpha}(\mathbf{r})$ it is $\Phi(-\mathbf{p})$.
- c) If $\langle \mathbf{S} \rangle$ is the expectation value of the spin angular momentum of the particle in the state $\Psi_{\alpha}(\mathbf{r})$ then in the motion-reversed state $\widetilde{\Psi}_{\alpha}(\mathbf{r})$ it is $-\langle \mathbf{S} \rangle$.
- d) By analyzing the appropriate Hamiltonian, discuss whether or not motion-reversal invariance holds for a spin-half charged particle that is subjected to
 - (i) a time-independent magnetic field;
 - (ii) a time-independent electric field;
 - (iii) a time-dependent electric field.

4) Antilinear and antiunitary operators – optional: Antilinear operators A act on ket vectors and operators O as follows:

$$\begin{aligned} c_1|\psi_1\rangle + c_2|\psi_2\rangle &\to & A\left(c_1|\psi_1\rangle + c_2|\psi_2\rangle\right) = c_1^*A|\psi_1\rangle + c_2^*A|\psi_2\rangle, \\ c_3 \,O &\to & A \, c_3 \, O \, A^{-1} = c_3^* \, A \, O \, A^{-1}. \end{aligned}$$

Note of the essential feature: the conjugation of the complex coefficients c_1 , c_2 , and c_3 .

To be antiunitary, an antilinear operator B must possess an inverse B^{-1} and leave the magnitude of any ket vector unchanged. Antiunitary operators can be expressed as products UK of standard unitary operators U and the important special case of an antilinear operator, the "complex conjugation only" operator K.

- a) By working in a complete and orthonormal but otherwise arbitrary basis show the following important properties of inner products and matrix elements under antiunitary transformations: If $|\psi'\rangle := B|\psi\rangle$, $|\phi'\rangle := B|\phi\rangle$, and $O' := BO'B^{-1}$, then
 - (i) $\langle \phi' | \psi' \rangle = \langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle;$
 - (ii) $\langle \phi' | O | \psi' \rangle = \langle \phi | O | \psi \rangle^* = \langle \psi | O^{\dagger} | \phi \rangle.$
- b) Consider the tunnelling of a particle through a potential barrier of arbitrary shape. Show that if the system is motion-reversal invariant, the probability of tunnelling between any two points is the same, regardless of the direction in which the tunnelling occurs. [Hint: You may wish to make use of the properties stated in part (a).]

The complex conjugation operator K, unlike a linear operator, depends on the basis in which its action is defined. For example, consider the two complete orthonormal bases $\{|a\rangle\}$ and $\{|\alpha\rangle\}$, along with the corresponding pair of complex conjugation operators, $K^{(a)}$ and $K^{(\alpha)}$, which are defined to act as follows:

$$\begin{aligned} K^{(a)}|\psi\rangle &= K^{(a)}\sum_{a}\psi_{a}|a\rangle := \sum_{a}\psi_{a}^{*}|a\rangle, \\ K^{(\alpha)}|\psi\rangle &= K^{(\alpha)}\sum_{\alpha}\psi_{\alpha}|\alpha\rangle := \sum_{\alpha}\psi_{\alpha}^{*}|\alpha\rangle. \end{aligned}$$

- c) Determine the condition on the relationship between the two bases such that $K^{(a)} = K^{(\alpha)}$. In particular, if the two bases differ merely by arbitrary phases $\{\phi_a\}$, so that $\{|\alpha\rangle = \exp i\phi_a |a\rangle\}$, state whether or not $K^{(a)} = K^{(\alpha)}$.
- d) Show that one can consistently obtain both the position and momentum eigenstate results $\mathcal{T}|\mathbf{r}\rangle = +|\mathbf{r}\rangle$ and $\mathcal{T}|\mathbf{p}\rangle = -|\mathbf{p}\rangle$ whether one works in the position or momentum basis.

Note again the conjugation feature, which is a characteristic of antilinear operators. Recall that for linear operators we were able to define their action to the left on bra vectors $\langle \psi |$ in a simple way. No such simple way structure can be developed for antilinear operators. For this reason, we shall assert that antilinear operators only act to the right, on ket vectors. Accordingly, we shall not introduce the notion of the adjoints of antilinear operators, including \mathcal{T} .

5) Applications of the motion-reversal operator – optional: The purpose of this question is to explore the motion-reversal formally, in terms of the motion reversal operator, and to explore some of the consequences of motion reversal. This topic, whose chief architect was Eugene P. Wigner (1902-1995), is usually referred to as *time reversal* but it should have been named *motion reversal*.

The motion-reversal operator \mathcal{T} is defined to be the operator that effects the transformation of any state $|\psi\rangle$ into the state $|\tilde{\psi}\rangle := \mathcal{T}|\psi\rangle$ in which motion is reversed. Repeating the time reversal operation restores the physical content of the original state, so that

 $\mathcal{T}\mathcal{T}|\psi\rangle = a \text{ phase factor } \times |\psi\rangle.$

Now, a theorem of Wigner's forces any such operator having this property to be either *unitary* or *antiunitary*. [We are already familiar with unitary operators (which are special cases of linear operators); antiunitary operators (which are special cases of antilinear operators) are less familiar, so we explore some of their properties in Question 4.] For reasons mentioned in Question 1, \mathcal{T} turns out to be antiunitary. Being antiunitary, \mathcal{T} can be expressed as UK, where U is a unitary operator and K is the complex conjugation operator discussed in Question 4.

a) By working in the position basis, show that the kinematic operators **R** and **P** transform under motion reversal so as to maintain the position **R** and reverse the momentum **P**:

$$\begin{array}{rcl} \mathbf{R} & \rightarrow & \mathbf{R}' = \mathcal{T} \, \mathbf{R} \, \mathcal{T}^{-1} = & \mathbf{R}, \\ \mathbf{P} & \rightarrow & \mathbf{P}' = \mathcal{T} \, \mathbf{P} \, \mathcal{T}^{-1} = -\mathbf{P}. \end{array}$$

[Note that spin, if present would also be reversed: $\mathbf{S} \to \mathbf{S}' = \mathcal{T} \, \mathbf{S} \, \mathcal{T}^{-1} = -\mathbf{S}$.]

- b) Show that these transformation properties guarantee that under motion reversal eigenstates of (i) position and (ii) momentum transform in the following natural ways: $|\mathbf{r}\rangle \rightarrow |\mathbf{r}\rangle$ and $|\mathbf{p}\rangle \rightarrow |-\mathbf{p}\rangle$.
- c) Show that motion reversal reverses the orbital angular momentum, i.e., $\mathbf{L} := \mathbf{r} \times \mathbf{p}$ transforms to $-\mathbf{L}$.
- d) Show that if A is antilinear and B is hermitian then

$$A\mathrm{e}^{-iB}A^{-1} = \mathrm{e}^{iABA^{-1}}.$$

e) Geometrical considerations indicate that the operations of spatial translation and rotation should be invariant under motion reversal. Use the result stated in part (d) to show that this invariance of translations and rotations dictates that the momentum and angular momentum operators **P** and **J** be reversed under motion reversal. [Note: The latter result is consistent with the notion that orbital and intrinsic angular momenta each is reversed under motion reversal.] f) Show that the fundamental commutators involving position and momentum, i.e.,

$$[R_{\mu}, P_{\nu}] = i\hbar\delta_{\mu\nu}$$

and, if present, spin, i.e., $[S_{\mu}, S_{\nu}] = i\hbar\epsilon_{\mu\nu\rho}S_{\rho}$ are preserved under motion reversal, provided that the condition $\mathcal{T} zI \mathcal{T}^{-1} = z^*I$ holds, where z is any complex c-number and I is the identity operator. Note that this is condition is consistent with \mathcal{T} being antiunitary.

- g) Determine how the orbital angular momentum \mathbf{L} (:= $\mathbf{R} \times \mathbf{P}$) transforms under motion reversal, and show that the orbital angular momentum commutator $[L_{\mu}, L_{\nu}] = i\hbar\epsilon_{\mu\nu\rho}L_{\rho}$ is thus preserved under motion reversal.
- h) The time-reversal operator does not explicitly transform the time variable in quantum mechanics t into the -t. Rather, show that if $|\psi(t)\rangle$ obeys the time-dependent Schrödinger equation, $i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$, and that if the Hamiltonian H is timereversal invariant so that $H \to H' = \mathcal{T} H \mathcal{T}^{-1} = H$, then $\mathcal{T} |\psi(-t)\rangle$ obeys the same Schrödinger equation. Note that one can also consider the issue of motion reversal from the perspective of the Heisenberg equations of motion for the position and momentum operators.

6) Motion-reversal-even and -odd systems:

- a) By expressing the motion-reversal operator \mathcal{T} as the product UK of a unitary operator U and the complex conjugation operator K, show that $\mathcal{T}^2 = \pm I$, where I is the identity operator. Systems for which $\mathcal{T}^2 |\Psi\rangle = +|\Psi\rangle$ are referred to as *even*; systems for which $\mathcal{T}^2 |\Psi\rangle = -|\Psi\rangle$ are referred to as *odd*. In this sense, systems containing an odd number of half-integral-spin particles are odd, regardless of the numbers of spinless or integer-spin particles they contain.
- b) Show that odd states and their motion-reversed counterparts are linearly independent.
- c) Show that the energy eigenstates of odd but motion-reversal-invariant systems are necessarily degenerate. This result is known as Kramers' theorem.
- d) For spinless particles motion reversal is equivalent to complex conjugation. As a consequence, the complex conjugate of any energy eigenstate of a motion-reversal-invariant system is an energy eigenstate having the same energy eigenvalue. Hence, show that nondegenerate energy eigenfunctions are real functions (up to an overall phase factor). [Note: One useful application of this result is that it can allow the narrowing—by almost a factor of two—of the number of parameters in a variational wave function.]