Physics 522. Quantum Mechanics II
Problem Set #4
Due Thursday, Mar. 3, 2011

Problem 1: Time Reversal Symmetry (10 Points)

The microscopic laws of physics are thought to be time reversal invariant. Loosely speaking this means the following. Suppose we take a movie of the motion of a system. If we run the movie backwards, could we tell?

In classical physics, Newton's Law

$$\frac{d^2\mathbf{x}}{dt^2} = -\nabla V(\mathbf{x})$$

is time-reversal in variant. That is if $\mathbf{x}(t)$ is a solution for given initial conditions at t=0, then $\mathbf{x}(-t)$ is a solution – that is the solution running backwards in time is also a solution.

In quantum physics (nonrelativistic, and ignoring spin), the dynamics can be described by the Schrödinger equation (e.g., for one particle),

$$\frac{\hbar}{-i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)\psi(\mathbf{x},t).$$

By inspection we see that given a solution $\psi(\mathbf{x},t)$, the function $\psi^*(\mathbf{x},-t)$ is also a solution. Thus the time reversed wave function in position space is the *complex conjugate*. We can thus define the time reversal operator by its action in position space,

$\hat{\Theta}|\psi\rangle = \hat{\Theta}\int d^3\mathbf{x}\,\psi(\mathbf{x})|\mathbf{x}\rangle = \int d^3\mathbf{x}\,\psi^*(\mathbf{x})|\mathbf{x}\rangle$ (complex conjugation in the basis $\{|\mathbf{x}\rangle\}$).

By this definition, $\hat{\Theta}^{-1} = \hat{\Theta}$.

(a) Show that $\hat{\Theta}$ is antiunitary.

(b) Use the position representation to show the following transformations for the position, momentum and orbital angular momentum operators.

$$\hat{\Theta}\hat{\mathbf{x}}\hat{\Theta}^{-1} = \hat{\mathbf{x}}\,,\quad \hat{\Theta}\hat{\mathbf{p}}\hat{\Theta}^{-1} = -\hat{\mathbf{p}}\,,\quad \hat{\Theta}\hat{\mathbf{L}}\hat{\Theta}^{-1} = -\hat{\mathbf{L}}\,.$$

We extend the time-reversal transformation on orbital angular momentum to include spin $\hat{\Theta}\hat{\mathbf{J}}\hat{\Theta}^{-1} = -\hat{\mathbf{J}}$, where $\hat{\mathbf{J}}$ is an arbitrary angular momentum operator.

(c) Show for spin 1/2 the time reversal operator can be written,

$$\hat{\Theta} = e^{-i\pi\hat{S}_y/\hbar}\hat{K}_z\,,$$

where $e^{-i\pi\hat{S}_y/\hbar}$ is the rotation operator about y by π, and $\hat{K}_z$ is complex conjugation in the standard basis (eigenstates of $\hat{S}_z$), i.e. this operator satisfies $\hat{\Theta}\hat{\mathbf{S}}\hat{\Theta}^{-1} = -\hat{\mathbf{S}}$.

Note, this division is not unique, so nothing is special about the y and z directions.

(d) Show that the Hamiltonian for the Hydrogen atom (including first order relativistic effects) is time-reversal invariant.

(e) Consider now adding an external magnetic field. Show that if all dynamics are time reversal invariant, that the electric and magnetic fields must transform as

$$\mathbf{E} \Rightarrow \mathbf{E} \text{ and } \mathbf{B} \Rightarrow -\mathbf{B}$$

Problem 2: Gauge Symmetry and the Aharonov-Bohm Effect (10 Points)
An important symmetry of physics, especially from the perspective of modern quantum field theory, is gauge invariance. Recall from the fundamental Hamiltonian for a charged particle q in a static electromagnetic field described by vector potentials **A** and electrostatic potential V is,

$$\hat{H} = \frac{1}{2m}\left|\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}(\hat{\mathbf{x}})\right|^2 + qV(\hat{\mathbf{x}})\,.$$

Under a "gauge-transformation" $\mathbf{A}(\mathbf{x}) \to \mathbf{A}(\mathbf{x}) + \nabla\chi(\mathbf{x})$ where χ is a scalar, the physical field **B** is unchanged. Thus, the quantum mechanical description must be gauge independent.

(a) Show that a gauge transformation is accomplished by the unitary transformation

$$\hat{U} = e^{-iq\chi(\hat{\mathbf{x}})/\hbar c}.$$

Thus show that under a gauge transformation, the wave function undergoes a phase shift, $\psi(\mathbf{x}) \to e^{-i\phi(\mathbf{x})}\psi(\mathbf{x})$, where $\phi(\mathbf{x}) = q\chi(\mathbf{x})/\hbar c$.

We can turn this argument on its head. Since we know that the physics must be invariant under a phase change of the wave function, and this phase can be position dependent, we MUST have gauge invariance. This is the fundamental theorem of modern field theory: Local phase change implies a "gauge field", here **A**.

(b) As an example, consider the charge localized at the origin. Expanding the scalar and vector potential in a Taylor series about the position of the charge gives the multipole expansion. Show that to up to the order of the electric dipole $\mathbf{d}$,

$$\hat{H} = \frac{1}{2m}\left|\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}(0)\right|^2 + \hat{\mathbf{d}} \cdot \nabla V(0) + \text{constant}.$$

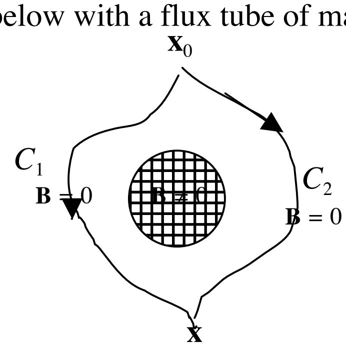
Perform a gauge transformation using the gauge function $\chi(\mathbf{x}) = -\hat{\mathbf{x}} \cdot \mathbf{A}(0)$, and show that the transformed Hamiltonian is

$$\hat{H}' = \frac{\hat{\mathbf{p}}^2}{2m} - \hat{\mathbf{d}} \cdot \mathbf{E}(0) + \text{constant}, \text{ where now } \mathbf{p} \text{ is usual kinetic momentum.}$$

This form of the Hamiltonian is much simpler and easier to interpret than the one above, though they are *physically equivalent*.

(c) Consider the function $\xi(\mathbf{x}) = \frac{q}{\hbar c}\int_{\mathbf{x}_0}^{\mathbf{x}} \mathbf{A}(\mathbf{x}) \cdot d\mathbf{l}$, where $\mathbf{x}_0$ is an arbitrary point and the integral is take over some path C connecting $\mathbf{x}$ and $\mathbf{x}_0$. Show that if $\psi_0(\mathbf{x})$ satisfies the *free* particle Schrödinger equation, $e^{i\xi(\mathbf{x})}\psi_0(\mathbf{x})$ is the solution in the presence of a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$.

(d) Show that $\xi(\mathbf{x})$ is not uniquely specified by $\mathbf{x}$, but also the *path C*. To do this, consider the two paths sketched below with a flux tube of magnetic field threading them.



Show that the *phase difference* accumulated by an electron along these two paths is

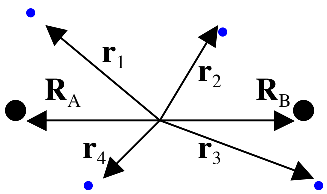
$$\Delta\phi_{12} = 2\pi\frac{\Phi}{\Phi_0},$$

where $\Phi = \int_S \mathbf{B} \cdot d\mathbf{a}$ is the magnetic field flux through a surface bounded by the closed loop, and $\Phi_0 = \frac{hc}{e}$ is the fundamental flux quantum (cgs units). This is amazing! It says that even though the electron travels only through regions of *strictly zero* magnetic field, so that classically there is **NO** Lorentz force, quantum mechanically the wave function is effected. This a *nonlocal global* property of the wave function, depending on the topology of the space. The two paths interfere, as has been observed. This is known as the Aharonov-Bohm effect.

Problem 3: Diatomic Molecule (10 points)

The simplest molecule consists of identical nuclei plus electrons. The basic features of the spectrum can be understood by considering the symmetries.

In the Born-Oppenheimer approximation, we take the nuclei as fixed and calculate the wavefunction of the electrons. These electronic states then determine a "molecular potential", in which the nuclei can move.



The Hamiltonian for the system can be written

$$\hat{H} = \sum_i \left(\frac{\hat{p}_i^2}{2m} - \frac{Z_A e^2}{|\hat{\mathbf{r}}_i - \mathbf{R}_A|} - \frac{Z_B e^2}{|\hat{\mathbf{r}}_i - \mathbf{R}_B|} \right) + \sum_{i \neq j} \frac{e^2}{|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|}.$$

(a) Show that this Hamiltonian is invariant under the following symmetries.
- (i) Continuous rotation about the internuclear axis.
- (ii) Parity (inversion of all coordinates through the center of the molecule).
- (iii) Reflection through a plane containing the internuclear axis.

(Note: there are also important exchange symmetries for the identical particles).

Now take Z_A=Z_b. If we take the internuclear axis to be the quantization axis, then these electron states have eigenvalue M of total electron angular momentum $\hat{L}_z$. Since, the direction of the axis (A-->B) or (B-->A) is irrelevant, the state depends only on $|M| \equiv \Lambda$, where Λ=0,1,2, are denoted Σ,Π,Δ,... (the Greek versions of the usual spectroscopic labels for atoms).

The parity eigenvalue p is denoted +1=g (gerade), -1=u (ungerade), using the German for even and odd. Thus we denote this electron states as Λ_p ("term" notation).

(b) Show that under symmetry (iii) $M \to -M$, and since the state depends only on $|M|$, prove that states with Λ>0 are doubly degenerate. In contrast, for Λ=0, the state is unchanged by a reflection and thus this degeneracy is broken. The Σ thus have must respect the reflection symmetry, with eigenvalue ±1. The Λ=0 states are denoted Σ_p^+ or Σ_p^-.

(c) When the nuclei are sufficiently separated compared to the size of an atom (order Å), the potential should asymptote to the energy of two free atoms. Consider then the Cl_2 molecule. Given that ground state Cl atoms have total electron angular momentum L=1 (i.e. P states), what are the possible molecular terms?