QUANTUM MECHANICS
Homework Set 9
April 17, 2014

1. Consider a particle of charge q moving with velocity $\mathbf{v}$ through electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$. The classical Hamiltonian is

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\Phi \ ,$$

where $\mathbf{A}$ is the vector potential and Φ is the scalar potential. The fields are given by $\mathbf{E} = -\nabla\Phi - \partial\mathbf{A}/\partial t$ and $\mathbf{B} = \nabla \times \mathbf{A}$.

In quantum mechanics, the Schrödinger equation is

$$H\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial t} \ ,$$

where the quantum mechanical Hamiltonian is obtained from the classical Hamiltonian by making the usual substitution, $\mathbf{p} \to -\mathrm{i}\hbar\nabla$. Then the Schrödinger equation becomes

$$\left[\frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\nabla - q\mathbf{A}\right)^2 + q\Phi\right]\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial t} \ .$$

(a) Show that the classical fields $\mathbf{E}$ and $\mathbf{B}$ are invariant under the gauge transformation,

$$\begin{aligned} \Phi' &= \Phi - \tfrac{\partial\Lambda}{\partial t} \ , \\ \mathbf{A}' &= \mathbf{A} + \nabla\Lambda \ , \end{aligned}$$

where Λ is an arbitrary differentiable function of space and time.

(b) The theory in quantum mechanics should also be invariant under gauge transformations. Show that

$$\psi' = \psi\mathrm{e}^{\mathrm{i}q\Lambda/\hbar}$$

is a solution of the Schrödinger equation,

$$\left[\frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\nabla - q\mathbf{A}'\right)^2 + q\Phi'\right]\psi' = \mathrm{i}\hbar\frac{\partial\psi'}{\partial t} \ .$$

2. In class, we discussed the ground state of the helium atom. If we ignore the repulsive Coulomb interaction between the two electrons, the ground state wave function would be

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \psi_{100}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2) = \frac{8}{\pi a_0^3} \mathrm{e}^{-2(r_1+r_2)/a_0} ,$$

and its energy would be

$$E_0 = 8(-13.6 \text{ eV}) = -109 \text{ eV} .$$

According to first-order perturbation theory, the lowest-order correction to E_0 is given by

$$V_{ee} = \frac{e^2}{4\pi\epsilon_0} \langle \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \rangle ,$$

where

$$\langle \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \rangle = \langle \psi_0 | \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} | \psi_0 \rangle$$

is the expectation value of the electron-electron interaction term with respect to the unperturbed ground-state wave function.

Calculate this expectation value and show that it equals $5/4a_0$. Evaluate V_{ee} in electron volts to find the corrected energy ($E_0 + V_{ee}$) for the ground-state energy. Compare with the experimental value.

Hint: Choose the z axis along $\mathbf{r}_1$ so that $|\mathbf{r}_1 - \mathbf{r}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}$ and then do the $d^3\mathbf{r}_2$ integral first. The θ_2 integral is easy but be careful to take the *positive root*. You'll have to break the r_2 integral into two pieces, one ranging from 0 to r_1 and the other ranging from r_1 to infinity.