MS 131, Problem Set #3

assigned 10/13/05
due 10/19/05

1. Show that an antisymmetric wave function results in particles that obey Pauli's exclusion principle [that is, no two particles can be in the same quantum state], whereas a symmetric wave function does not. In each case you will need to write down a total wave function for two particles. The symmetry of the wave function is defined with respect to the exchange of the position of the particles.

2. Consider two Fermions in an unspecified potential well (could be an infinite square well potential, could be the potential about a helium nucleus). Let $\psi_\alpha(r)$ be the wave function for a single Fermion in that well.

   (a) Write down $\psi^T(r_1,r_2)$ as a Slater determinant, and then also in algebraic form.

   (b) What assumption has been made in writing down this type of wave function for the total system?

   (c) Show that this wave function satisfies (i) the requirement that the particles be indistinguishable, and (ii) the Pauli exclusion principle.

   (d) The wave function of part (a) can also be written as a multiple of the total position wave function and the total spin wave function. Using this form of the total wave function, show that Fermions with parallel spin 'repel' and those with antiparallel spin 'attract.' Assume without proof that if the total spin wave function is symmetric, the spins of the two Fermions are parallel, and, similarly, if the total spin wave function is antisymmetric, the spins are antiparallel.

3. The angular momentum, $\vec{L}$, of a moving particle, with respect to some origin, is defined as $\vec{r} \times \vec{p}$, where $\vec{r}$ is the vector distance between the particle and the origin, and $\vec{p}$ is the momentum.

   (a) Write down the quantum mechanical operator $\hat{L}$, that is analogous to the classical quantity, $\vec{L}$.

   It can be shown that in spherical coordinates, the operator that gives the z-component of angular momentum is given by

   $$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}.$$

   (b) Using this definition, show that, for the hydrogen atom:

   $$\left\langle \hat{L}_z \right\rangle = L_z = \hbar m_l .$$

4. Write down the total Hamiltonian for the helium atom, which has one nucleus and two electrons. Define the vector between the nucleus and the electrons as $\vec{r}_1$ and $\vec{r}_2$, respectively. Why is it not possible to solve for the wave function analytically? What mathematical technique are we unable to use?

5. Consider the H_2^+ molecular ion in the ground state. Evaluate the overlap integral, *S*, using the 1s wavefunctions (given in dimensionless spatial coordinates, $r_A = \mathbf{r_A}/a_0$, where a_0 = the Bohr radius, as)

$\psi_{1s}(r_A) = \pi^{-½} \exp(-r_A)$; $\psi_{1s}(r_B) = \pi^{-½} \exp(-r_B)$

Hint: transform the coordinate system to $\mu = (r_A + r_B)/R$ and $\eta = (r_A - r_B)/R$ where R is the internuclear distance.

The volume integral in these coordinates is $dV = R^3/8\,(\mu^2 - \eta^2)d\mu d\eta d\phi$. The integration limits are μ: $1 \rightarrow \infty$; η: $-1 \rightarrow +1$; ϕ: $0 \rightarrow 2\pi$

Hint: $\int_1^\infty x^n \exp(-ax)dx = \frac{n!\exp(-a)}{a^{n+1}} \sum_{k=0}^{n} \frac{a^k}{k!}$