

PHYS-4601 Homework 12 Due 16 Jan 2014

This homework is due in the dropbox outside 2L26 by 11:59PM on the due date. If you wish to turn it in ahead of time, you may email a PDF or give a hardcopy to Dr. Frey.

1. 3-Particle States *a mix of Griffiths 5.7 and 5.33*

Consider three particles, each of which is in one of the single-particle states $|\alpha\rangle$, $|\beta\rangle$, or $|\gamma\rangle$, which are orthonormal.

- If the particles are bosons, write down the state where one particle is in each of $|\alpha\rangle$, $|\beta\rangle$, and $|\gamma\rangle$. *Hint:* This state must be symmetric under the exchange of *any* pair of the bosons.
- Write down all possible 3-particle states (including normalization) with two particles in the same 1-particle state and the third particle in a different 1-particle state.
- How many linearly independent states can you form if the particles are fermions? Write down all the possible linearly independent states. *Hint:* Similarly to the above, these states must be antisymmetric under the exchange of *any* pair of the fermions.

2. Hydrogen Molecule

The electrons in a molecule are tightly bound and provide a potential for the motion of the nuclei. For a diatomic molecule, it is often a good approximation to expand the potential around the equilibrium separation r_0 as

$$V(r) = V_0 + \frac{1}{2}m\omega^2(r - r_0)^2, \quad (1)$$

ignoring other terms, where $V_0 < 0$, ω is a characteristic frequency, and m is the reduced mass of the two nuclei. We ignore other terms in the expansion.

- Find the energy eigenvalues for bound states of the nuclear motion of this diatomic molecule. When you consider the rotational motion, you can assume that the radial potential is so steep that the radius is fixed at $r = r_0$.
- Consider an H_2 molecule, so that the two nuclei are identical particles (protons). If the nuclear spins are in a total spin singlet state, what values of the orbital angular momentum quantum numbers are allowed? Note that exchanging the two nuclei is equivalent to taking $\vec{x} \rightarrow -\vec{x}$ in the spatial wavefunction, which is $r \rightarrow r$, $\cos\theta \rightarrow -\cos\theta$, $\phi \rightarrow \phi + \pi$ in spherical polar coordinates.
- Including the nuclear orbital angular momentum and electron spin, are H_2 molecules fermions or bosons?

3. Estimating Helium Better *Griffiths 5.11 clarified*

In this problem, we will estimate the ground state energy of a helium atom. We will imagine that the electron repulsion is a correction to the attraction between the electrons and the nucleus.

- Consider the states of a single electron around a helium nucleus (which has twice the charge of a proton). Argue that the “helium Bohr radius” $a_{\text{He}} = a/2$, where a is the usual Bohr radius, and that therefore the single-electron ground state wavefunction is given by

$$\langle \vec{x} | n = 1, \ell = 0, m = 0 \rangle = \sqrt{\frac{8}{\pi a^3}} e^{-2r/a}. \quad (2)$$

Next assume that the two electron helium groundstate is $|n = 1, \ell = 0, m = 0\rangle_1 |n = 1, \ell = 0, m = 0\rangle_2 |s = 0, m_s = 0\rangle$, where the total spin state is the antisymmetric singlet. (The spatial wavefunction is given by Griffiths eqn [5.30].) Briefly argue that the energy of this state, in the absence of electron repulsion, is given by Griffiths eqn [5.31].

(b) Now find $\langle |\vec{x}_1 - \vec{x}_2|^{-1} \rangle$ in this state, as follows:

1. Use the trick of setting the z axis for \vec{x}_2 along \vec{x}_1 and the law of cosines to see

$$|\vec{x}_1 - \vec{x}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1r_2 \cos \theta_2}.$$

2. Do the angular integrals for \vec{x}_2 , noting that

$$\int_0^\pi d\theta \sin \theta f(\cos \theta) = \int_{-1}^1 dx f(x).$$

Your result will have square roots of perfect squares, which are equal to absolute values. *Be careful of that!*

3. Carry out the r_2 integral in two parts, $0 < r_2 \leq r_1$ and $r_1 < r_2 < \infty$.

4. Now do the \vec{x}_1 integrals.

Hint: The “exponential integrals” formula in the back cover of Griffiths will be helpful.

(c) Estimate the change in the ground state energy due to the electron repulsion as

$$\Delta E = \frac{e^2}{4\pi\epsilon_0} \left\langle \frac{1}{|\vec{x}_1 - \vec{x}_2|} \right\rangle. \quad (3)$$

Write ΔE in terms of the Bohr radius a and estimate its value in eV. Then add this to the energy from part (a) to get a rough estimate of the He ground state energy. *Hint:* Remember that the hydrogen ground state energy is $-\hbar^2/2ma^2 = -13.6$ eV.