Physics 487 – Homework #8 due Friday Oct 23 @ midnight: 1 file → my.physics Course Uploads

You may use anything from the **486/7 formula sheets** without derivation
… but do try to see how far you can get on your own on your Desert Island. ☺
You may also use **wolframalpha**.com or similar tool to evaluate your integrals
after you set the up in a form that can be **directly entered** into such tools.

Problem 1 : Variational Principle : 1D SHO *adapted from Griffiths 7.12*

(a) Find the best bound on the ground state energy, E_{gs}, of the 1D SHO ™ using a trial wavefunction of the form

$$\psi(x) = \frac{A}{\left(x^2+b^2\right)^n}.$$

for arbitrary n (i.e. n is supposed to be a given value, not a free parameter, but it is not restricted to integers). Many hints now follow to help you manage this calculation, please read them first:

▶ Find the optimal value of the variational parameter b but **DO NOT** find the optimal value of the other variational parameter n. Leave n in your answers, as part (c) addresses the variation of n.

▶ Lots of integration to do, please DO use **wolframalpha**. You will need the following integral repeatedly, and wolframalpha annoyingly won't do it, so please use this formula freely :

$$\int_0^\infty \frac{x^k}{\left(x^2+b^2\right)^a}dx = \frac{1}{2b^{2a-k-1}}\frac{\Gamma\left(\frac{k+1}{2}\right)\Gamma\left(\frac{2a-k-1}{2}\right)}{\Gamma(a)}$$

Also check out **integral-calculator.com**, which *can* do the previous integral. It comes out in terms of beta functions $B(x,y)$ which are "Euler beta functions" if you want to pick them out from the many other "beta functions" in math and physics.

▶ Lots of **Γ functions** about. For this question all you need to evaluate are ratios of Γ functions, and in that context this well-known relation is all you need:

$$\Gamma(n) = (n-1)! \quad \text{or the recursive version,} \quad \Gamma(n) = (n-1)\Gamma(n-1) = (n-1)(n-2)\Gamma(n-2) = \ldots$$

Don't worry about the values of Γ(½) and such, you can look all of that up if you want. Just keep the Γ functions as is until *all* of your integrals are done, then you will see that many of them cancel, and all you need are *ratios* of Γ functions *whose arguments are separated by integers*. Those are all doable with $\Gamma(n)=(n-1)!$ For example, $\Gamma(9/2) / \Gamma(5/2) = (7/2)! / (3/2)! = 7/2 \cdot 5/2 = 35/4$. If you look in the checkpoints file, you will find an intermediate checkpoint that shows the expression you should get after all the gamma functions are gone.

(b) Find the lowest upper bound on the first excited state of the harmonic oscillator using a trial wavefunction of the form

$$\psi(x) = \frac{Bx}{\left(x^2+b^2\right)^n}.$$

To save you from having to do the same integration as you did in part (a), **start from here** :

$$\langle T\rangle = \frac{3\hbar^2}{4mb^2}\frac{n(4n-3)}{(2n+1)} \quad \text{and} \quad \langle V\rangle = \frac{3}{2}\frac{m\omega^2 b^2}{(4n-5)}$$

when the new trial wavefunction is used.

(b′) Why does the trial wavefunction you used in part (b) give you an upper limit on the first-excited state whereas the trial function from part (a) gave you an upper limit on the ground state? A brief but clear qualitative answer is what we're looking for, no calculations necessary.

(c) It is clear by inspection of your part (a) and (b) results that the variational-method energies of the ground state and first excited state reach the exact SHO values in the limit $n \to \infty$. (If it is not obvious by inspection, please ask!) Why do we get such perfect results? To find out, show that the trial wavefunctions from parts (a) and (b) approach the exact SHO wavefunctions in the limit $n \to \infty$.

▶ You will need **Stirling's approximation**: $\ln(z!) \approx z\ln(z) - z$ for $z >> 1$. The exponential of that relation will allow you to work with the factorial $z!$ in the limit $z \to \infty$.

Problem 2 : On the nature of Helium, Screening, and Effective Charge

Griffiths' section §7.2 goes through the most CLASSIC application of the variational principle: finding the ground state energy of the helium atom including the mutual Coulomb repulsion between the two electrons. When we discussed **screening** in our atomic structure section, we advertised that we would come back to the concept of an effective nuclear charge < Z and calculate one when we had more tools. Well here we are!

First, here is a summary of Griffiths §7.2. The Hamiltonian used for the helium atom is :

$$H(\vec{r}_1,\vec{r}_2) = -\frac{\hbar^2}{2m}\left(\nabla_1^2+\nabla_2^2\right) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{2}{r_1}+\frac{2}{r_2}-\frac{1}{|\vec{r}_1-\vec{r}_2|}\right)$$

No spin-dependent forces here, just the Coulomb attraction of each electron to the Z_{He}=2 nucleus and the electron-electron repulsion term (which we call V_{ee} for short). The trial wavefunction used for this classic problem is essentially the product of two hydrogen wavefunctions, one for each of helium's electrons:

$$\psi(\vec{r}_1,\vec{r}_2) = \frac{Z^3}{\pi a_0^3} e^{-Z(r_1+r_2)/a_0}$$

where a_0 is the Bohr radius (see 486 formula sheet).

"Wait", you remark, "if a_0 is the Bohr radius, that trial wavefunction has no variable parameter, I thought we were always supposed to include at least one in order to minimize our ground-state energy as much as possible?" You are correct … and there *is* a variable parameter: it is Z. "But $Z = 2$ for Helium!", you exclaim, "I can't play around with the truth!" True … but the idea behind this trial wavefunction is to introduce an **effective *Z*** that will come out *less* than $Z_{He} = 2$ because the effect of the V_{ee} term is to partially **screen the nuclear charge**. To understand, imagine you are one of the two electrons and that your name is Ivan. You are attracted to the positively-charged $Z_{He} = 2$ nucleus, which sits at the center of your probabilistic cloud of spherically-symmetric *s*-shell existence ... but you are repelled by the other electron, named Juan, which is probabilistically splattered through space the same way you are. If you think about Juan using your mastery of Gauss' Law from PHYS 212 (footnote available[1]), you will realize the following: if you, Ivan, are momentarily located a distance r_{ivan} away from the nucleus, the *only* portion of Juan's probability cloud that affects you is the part that is closer to the nucleus than you are, i.e. the part with $r_{juan} < r_{ivan}$. Juan is negatively charged, as are you, so the electric field you see at your location is due to attraction from the charge $+Z_{He}$ nucleus & repulsion from a portion of Juan's charge –1 cloud. Thus, Juan **screens** part of the $+Z_{He}$ nuclear charge from you. Our

[1] From Gauss' Law: the electric field $E(r)$ at a distance r from the center of a spherically symmetric charge distribution is $Q_{enc}(r)/4\pi\varepsilon_0 r^2$ where $Q_{enc}(r)$ stands for the total charge **enclosed within the distance *r***. None of the charge outside the radius r affects the electric field $E(r)$ at all. Another way to put this is that a spherically symmetric **shell** of charge produces **zero E-field** everywhere inside the empty spherical hole in the middle. That is a fairly AMAZING result from Gauss' Law, actually … think of all the cancellations of all the little field vectors at every point in the empty core that has to occur … symmetry, dude, wow.

hope is that introducing an effective = screened charge Z as a variational parameter will provide a good approximation to the full effect of the V_{ee} term.

As you see in Griffiths, the best values obtained for the He ground state using the "(hydrogen)^2-with-screening" trial function are $Z = 1.69$ (which is less than 2, so yes, the helium nucleus is screened in this model) and $E_{gs} = -77.5$ eV. This is absurdly close to the experimental value of **–79 eV**. You may recall that in a previous homework, you used 1st order perturbation theory to calculate the very same thing – the effect of V_{ee} on the helium ground state energy – and you obtained $E_{gs} = -75$ eV. That's not quite as good, but of course with perturbation theory, you can keep going, to 2nd order, 3rd order, etc with enough time/energy/processors.

(a) The "(hydrogen)^2-with-screening" trial function does NOT do such a good job in obtaining the ground state of the **H^- ion**, i.e. a hydrogen nucleus surrounded by two electrons in a closed $1s^2$ shell. Using the trial wavefunction described above, calculate the approximate ground state energy of the H^- ion with V_{ee} repulsion included.

▶ To shorten this problem, you may use any result from Griffiths §7.2, just give the equation number.

▶ FYI: It is very common in atomic calculations, such as this one, to need $< 1/r >$ and/or $< 1/r^2 >$ for hydrogenic wavefunctions ψ_{nlm}. The answers are equations 6.55 and 6.56 in Griffiths, and you are free to use them, but I do want you to know that there is a very fast way to get the first one. You use the super-useful Virial Theorem, which is true in both QM and CM: $<V> = -2<T>$ for a particle bound in a $1/r$ potential. Since you know $<E> = <T+V>$ for the hydrogenic wavefunctions (well, it's on your formula sheet) and $V \sim 1/r$, $< 1/r >$ is easily obtained! This is problem 6.12 in Griffiths; the calculation of $< 1/r^2 >$ is addressed in problem 6.33 & 6.32, which is a bit of a project.

(b) Let's leave the H^- ion alone for a moment and jargon-bust the word **ionization**. It means "the freeing of an electron from an atomic bound state". Remember that to **free** a bound particle means to elevate its total energy from a negative value (its bound-state energy) to ZERO, at which point it is able to reach ∞ = a place free of influence from any other forces (V=0) with just enough kinetic energy to be physical (T=0).
Consider the **He^+ ion** = a helium atom with one electron removed. As noted above, a He atom has ground state energy –79 eV; calculate the **ionization energy** required to free one electron from a ground-state He atom and turn it into a ground-state He^+ ion.

▶ Massive hints: (i) consult the 486 formula sheet, and (ii) this is a very short problem.