Week 8 Worksheet Solutions
Variational Principle

Jacob Erlikhman

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Exercise 1. Prove the variational principle,

$$E_{\text{gs}} \leq \langle\psi|H|\psi\rangle.$$

This is in Griffiths.

Exercise 2. Use the variational principle to get an approximation for the ground state energy in the **Yukawa potential**

$$V(r) = e^{-\alpha r}\frac{e^2}{r},$$

using the trial function

$$\psi(r) = \sqrt{\frac{b^3}{\pi}}e^{-br}.$$

Show that when $\alpha = 0$, the trial function saturates the bound; why? Comment on the accuracy of the bound you obtain as α increases. Note that

$$\nabla^2 f(r) = \frac{1}{r^2}\partial_r(r^2\partial_r f(r)).$$

Note that we don't need to consider any angular part to our wavefunction, because if we're approximating the ground state energy, we know that will always be in an $\ell = 0$ state. Indeed, the Yukawa potential is just a screened Coulomb potential; in the Coulomb potential, the $\ell = 0$ states are always lower energy than the $\ell > 0$ states (for fixed n). Thus, $\psi(r)$ is our total wavefunction. Now,

$$\nabla^2\psi = \partial_r{}^2\psi + \frac{2}{r}\partial_r\psi = (b^2 - 2b/r)\psi.$$

We can then evaluate

$$\langle H\rangle = \left\langle -\frac{\hbar^2}{2m}\nabla^2 + V(r)\right\rangle = \frac{4\pi b^3}{\pi}\left[-\frac{\hbar^2}{2m}\int_0^\infty (b^2r^2 + br)e^{-2br}\,\mathrm{d}r + e^2\int_0^\infty re^{-(2b+\alpha)r}\,\mathrm{d}r\right].$$

In order to evaluate these integrals, we need to use the identity

$$\int_0^\infty r^n e^{-ar}\,\mathrm{d}r = \frac{n!}{a^{n+1}},$$

which you can prove by using induction and integration by parts. We thus get

$$\begin{aligned}\langle H\rangle =& 4b^3\left[-\frac{\hbar^2}{2m}\left(\frac{1}{4b}+\frac{1}{4b}\right)+\frac{e^2}{(2b+\alpha)^2}\right]\\ =& -\frac{\hbar^2 b^2}{2m}+\frac{4e^2b^3}{(2b+\alpha)^2}.\end{aligned}$$

We want to minimize this with respect to b, so we should solve

$$\partial_b \langle H\rangle = 0.$$

This gives

$$0 = \frac{b\hbar^2}{m} - \frac{12b^2e^2}{(2b+\alpha)^2} + \frac{16e^2b^3}{(2b+\alpha)^3}.$$

Note that after multiplying out by $(2b+\alpha)^3$, we can factor out one factor of b to get a cubic equation for b (plus a spurious $b = 0$ solution), which unfortunately is not analytically tractable (sorry!). On the other hand, when $\alpha = 0$, this drastically simplifies to

$$0 = \frac{b\hbar^2}{m} - 3e^2 + 2e^2,$$

from which it follows that

$$b = \frac{e^2 m}{\hbar^2}.$$

Plugging this back in to $\langle H\rangle$, we find

$$\langle H\rangle = -\frac{e^4m^2}{2\hbar^2},$$

which is exactly the first Bohr energy (in gaussian units)! This makes sense, since if $\alpha = 0$, the potential is just the Coulomb potential, and our wavefunction is just $\psi(r) = R_{n0}(r)$! So we expect that as we turn on α, the approximation we get to the energy will get worse and worse, since the true ground state wavefunction will be farther and farther away from what we wrote down, which is basically just $R_{n0}(r)$.