Physics 443, Solutions to PS 10

1. **Griffiths 7.13**

Normalize so that

$$\begin{aligned} 1 &= 4\pi \int_0^\infty |\psi|^2 r^2 dr = 4\pi |A|^2 \int_0^\infty e^{-2br^2} r^2 dr \\ &= 4\pi |A|^2 \sqrt{\pi} 2 \left(\frac{1}{2\sqrt{2b}} \right)^3 \\ &\rightarrow \ A = \left(\frac{2b}{\pi} \right)^{\frac{3}{4}} \end{aligned}$$

Let $u(r) = r\psi(r) = Are^{-br^2}$ and the Hamiltonian is

$$\begin{aligned} Hu(r) &= \frac{d^2u}{dr^2} + \frac{2m}{\hbar^2} \frac{e^2}{4\pi\epsilon_0 r} u \\ &= A\frac{d}{dr}(1 - 2br^2)e^{-br^2} + A\frac{2m}{\hbar^2}\frac{e^2}{4\pi\epsilon_0}e^{-br^2} \\ &= A(-4br - 2br + 4b^2r^3)e^{-br^2} + A\frac{2m}{\hbar^2}\frac{e^2}{4\pi\epsilon_0}e^{-br^2} \end{aligned}$$

The energy

$$\begin{aligned} \langle u \mid H \mid u \rangle &= 4\pi \frac{\hbar^2}{2m} |A|^2 \int_0^\infty \left[(-6br^2 + 4b^2r^4)e^{-2br^2} + \frac{2m}{\hbar^2}\frac{e^2}{4\pi\epsilon_0} re^{-2br^2} \right] dr \\ &= 4\pi \frac{\hbar^2}{2m} \sqrt{\pi} |A|^2 \left[-\frac{12b}{8(2b)^{\frac{3}{2}}} + \frac{48b^2}{32(2b)^{\frac{5}{2}}} + \frac{m}{\hbar^2}\frac{e^2}{4\pi\epsilon_0}\frac{1}{(2b\sqrt{\pi})} \right] \\ &= 4\pi \frac{\hbar^2}{2m} \sqrt{\pi} |A|^2 \left[-\frac{3}{4(2b)^{\frac{1}{2}}} + \frac{3}{8(2b)^{\frac{1}{2}}} + \frac{m}{\hbar^2}\frac{e^2}{4\pi\epsilon_0}\frac{1}{(2b\sqrt{\pi})} \right] \\ &= 4\pi \frac{\hbar^2}{2m} \sqrt{\pi} \left(\frac{2b}{\pi} \right)^{\frac{3}{2}} \left[-\frac{3}{8(2b)^{\frac{1}{2}}} + \frac{m}{\hbar^2}\frac{e^2}{4\pi\epsilon_0}\frac{1}{(2b\sqrt{\pi})} \right] \\ &= 4\pi \frac{\hbar^2}{2m\pi} \left[-\frac{6b}{8} + \frac{m}{\hbar^2}\frac{e^2}{4\pi\epsilon_0} \left(\frac{2b}{\pi} \right)^{\frac{1}{2}} \right] \end{aligned}$$

Then take the derivative with respect to b and set equal to zero to get b.

$$\begin{aligned} \frac{3}{4} &= \frac{m}{2\hbar^2}\frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{b\pi} \right)^{\frac{1}{2}} \\ &\rightarrow \ \sqrt{b} = \frac{2}{3}\frac{m}{\hbar^2}\frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}} \end{aligned}$$

Substitution back into the expression for the energy gives

$$\begin{aligned} E &= \frac{2\hbar^2}{m}\left[-\frac{3}{4}\frac{4}{9}+\frac{2}{3}\right]mc^2\alpha^2\frac{m}{\hbar^2}\frac{2}{\pi} \\ &= \frac{2}{3}2E_1\frac{2}{\pi} = 0.85E_1 \end{aligned}$$

2. **Griffiths 7.14** The goal is to use the variational principle for the Yukawa potential. We use the ground state of Hydrogen

$$\psi(a) = \sqrt{\frac{1}{\pi a^3}}e^{\frac{r}{a}}.$$

We need to calculate $\langle H\rangle = \langle T\rangle + \langle V\rangle$, where $\langle T\rangle = \frac{\hbar^2}{2m}\frac{1}{a^2}$ and $\langle V\rangle$ can be found after performing an integral. We can write the result as

$$\langle H(a)\rangle \leq -E_1\left[\left(\frac{a_0}{a}\right)^2 - 2\frac{a_0}{a}\left(\frac{1}{1+\mu a/2}\right)\right],$$

where E_1 is the ground state energy of Hydrogen, and a_0 is the Bohr radius. In this form, it is clear that if $\mu \to 0$, and $a \to a_0$, we reproduce the results for Hydrogen. Our Variational principle is to set $\partial_a\langle H\rangle = 0$. A little bit of algebra gives

$$\frac{a_0}{a} = \left(\frac{1}{1+\mu a/2}\right)^3\left(1+\frac{3}{2}\mu a\right) \approx 1 - \frac{9}{4}(\mu a)^2.$$

Substituting back, we find that

$$\begin{aligned} E &\leq -E1\left[1-\frac{9}{2}(\mu a)^2 - 2\left(1-\frac{9}{4}(\mu a)^2\right)\left(1-(\mu a)+\frac{3}{4}(\mu a)^2\right)\right], \\ &\leq E_1\left(1-2(\mu a)-\frac{3}{2}(\mu a)^2+\cdots\right). \end{aligned}$$

3. **Griffiths 7.15**

(a) We have the Hamiltonian

$$H = \begin{pmatrix} E_a & h \\ h & E_b \end{pmatrix},$$

which can be easily solved to give

$$\epsilon_{\pm} = \frac{E_a + E_b}{2} \pm \frac{1}{2}\sqrt{(E_a - E_b)^2 + 4h^2}.$$

To compare with other approximations, we can expand this exact result to the case if h is small

$$\epsilon_+ = E_a + \frac{h^2}{E_a - E_b},\ \epsilon_- = E_b - \frac{h^2}{E_a - E_b}.$$

(b) We see that first order perturbation theory gives 0, because our perturbation has no diagonal terms. And we can immediately write down the second order result

$$E_a^{(2)} = \frac{h^2}{E_a - E_b},\ E_b^{(2)} = \frac{h^2}{E_b - E_a}.$$

(c) We use the trial wavefunction $(\cos\phi, \sin\phi)$ to find that $\langle H(\phi)\rangle = E_a\cos^2(\phi) + E_b\sin^2(\phi) + h\sin(2\phi)$. We need that $\partial_\phi\langle H(\phi)\rangle = 0$, which gives us the condition that

$$\tan(2\phi) = \frac{-2h}{E_b - E_a} = \frac{\sin(2\phi)}{\cos(2\phi).}$$

Plugging back in, we have

$$\begin{aligned}
\langle H\rangle &= \frac{E_a}{2} + \frac{E_b}{2} + \frac{E_a - E_b}{2}\cos(2\phi) + h\sin(2\phi), \\
&= \frac{E_a + E_b}{2} - \frac{1}{2}\left(\frac{(E_a - E_b)^2 + 4h^2}{\sqrt{(E_a - E_b)^2 + 4h^2}}\right), \\
&= \frac{E_a + E_b}{2} - \frac{1}{2}\sqrt{(E_a - E_b)^2 + 4h^2}.
\end{aligned}$$

(d) If we expand the exact result to second order in h, it agrees with the result from second order perturbation theory. The variational method yields the exact energy since the trial wave function had the form of the exact solution.