Quantum Mechanics II
Assignment II

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1 Problem 7.11

Find the lowest bound on the ground state of hydrogen you can get using a gaussian trial wave function

$$\psi(\mathbf{r}) = Ae^{-br^2}, \tag{1.1}$$

where A is determined by normalisation and b is an adjustable parameter. *Answer:* -11.5 eV.

Solution:

First of all, let's write down the Hamiltonian for the Hydrogen

$$H_{Bohr} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{1.2}$$

Now, we have to follow the next steps to addres this problem

1. Normalise our trial wavefunction:

$$\begin{aligned}
1 = \langle\psi|\psi\rangle &= |A|^2 \int e^{-2br^2} r^2 sin\theta dr d\theta d\phi \\
&= |A|^2 \int_0^\infty e^{-2br^2} r^2 dr \underbrace{\int_0^\pi sin\theta d\theta \int_0^{2\pi} d\phi}_{4\pi} \\
&= |A|^2 4\pi \int_0^\infty e^{-2br^2} r^2 dr
\end{aligned}$$

   Using

$$\boxed{\int_0^{+\infty} r^m e^{-ar^2} dr = \frac{\Gamma\left(\frac{m+1}{2}\right)}{2a^{\frac{m+1}{2}}}} \tag{1.3}$$

$$1 = 4\pi|A|^2 \frac{1}{4}\sqrt{\frac{\pi}{(2b)^3}} = |A|^2\left(\frac{\pi}{2b}\right)^{3/2}$$

$$\Rightarrow A = \left(\frac{2b}{\pi}\right)^{3/4} \tag{1.4}$$

2. Compute $\langle\psi|\hat{T}|\psi\rangle$

$$\langle\psi|\hat{T}|\psi\rangle = \int \psi\left(-\frac{\hbar^2}{2m}\nabla^2\psi\right) dr\, sin\theta\, d\theta\, d\phi \tag{1.5}$$

Firs we need to compute

$$\begin{aligned}\nabla^2\psi(\mathbf{r}) &= \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\psi\right), \quad \text{no angular dependence!}\\ &= A\frac{1}{r^2}\frac{d}{dr}\left(-2b\, r^3\, e^{-2br^2}\right)\\ &= -2b\, A\frac{1}{r^2}\left(3r^2 - 2r^4\right) e^{-2br^2}\\ &= \frac{-2b}{r^2}\left(3r^2 - 2r^4\right)\psi(\mathbf{r})\end{aligned} \tag{1.6}$$

Then, Equation 1.5 becomes

$$\langle\psi|\hat{T}|\psi\rangle = -\frac{\hbar^2}{2m}|A|^2(-2b)4\pi\int_0^\infty \left(3r^2 - 2br^4\right) e^{-2br^2} dr \tag{1.7}$$

We can solve the integral using Equation 1.3, then

$$\begin{aligned}\langle\psi|\hat{T}|\psi\rangle &= \frac{4\hbar^2\pi\, b}{m}\left(\frac{2b}{\pi}\right)^{3/2}\left[3\frac{1}{8b}\sqrt{\frac{\pi}{2b}} - 2b\frac{3}{32b^2}\sqrt{\frac{\pi}{2b}}\right]\\ &= \frac{4\hbar^2\pi\, b}{m}\left(\frac{2b}{\pi}\right)\left(\frac{3}{8b} - \frac{3}{16b}\right)\\ &= \frac{4\hbar^2\pi\, b}{m}\left(\frac{2b}{\pi}\right)\left(\frac{3}{16b}\right) = \boxed{\frac{3\hbar^2\, b}{2m} = \langle\hat{T}(b)\rangle}\end{aligned} \tag{1.8}$$

3. Compute $\langle\psi|\hat{V}|\psi\rangle$

$$\begin{aligned}\langle\psi|\hat{V}|\psi\rangle &= -\frac{e^2}{4\pi\epsilon_0}|A|^2 4\pi\int_0^\infty e^{-2br^2}\frac{1}{r}r^2\, dr\\ &= -\frac{e^2}{4\pi\epsilon_0}\left(\frac{2b}{\pi}\right)^{3/2}\left(\frac{4\pi}{4b}\right)\\ &= \boxed{-\frac{e^2}{4\pi\epsilon_0}2\sqrt{\frac{2b}{\pi}} = \langle\hat{V}(b)\rangle}\end{aligned} \tag{1.9}$$

4. Compute $\langle\hat{H}\rangle = \langle\hat{T}(b)\rangle + \langle\hat{V}(b)\rangle = E_{gs}(b)$

   Using the results from Equation 1.8 and Equation 1.9 write

$$\langle\hat{H}\rangle = \frac{3\hbar^2\, b}{2m} - \frac{e^2}{4\pi\epsilon_0}2\sqrt{\frac{2b}{\pi}} = E_{gs}(b) \tag{1.10}$$

5. Now, we need to minimise $E_{gs}(b)$

$$\frac{\partial}{\partial b}E_{gs}(b) = \frac{3\hbar^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{b}} = 0 \tag{1.11}$$

solving for b

$$\sqrt{b} = \frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}}\left(\frac{2m}{3\hbar^2}\right) \Rightarrow b_{min} = \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{2}{\pi}\left(\frac{2m}{3\hbar^2}\right)^2 \tag{1.12}$$

Replacing the result from Equation 1.12 into Equation 1.10 we get

$$\begin{aligned} E_{gs}(b_{min}) &= \frac{3\hbar^2}{2m}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{2}{\pi}\frac{4m^2}{9\hbar^4} - \frac{e^2}{4\pi\epsilon_0}2\sqrt{\frac{2}{\pi}}\frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}}\left(\frac{2m}{3\hbar^2}\right) \\ &= \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{m}{\hbar^2}\left(\frac{4}{3\pi} - \frac{8}{3\pi}\right) \\ &= \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{m}{\hbar^2}\left(-\frac{4}{3\pi}\right) \\ &= -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\left(\frac{8}{3\pi}\right), \quad E_1 = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \\ &= \boxed{\frac{8}{3\pi}E_1 = \frac{8}{3\pi}(-13.6\,eV) = -11.5\,eV} \end{aligned} \tag{1.13}$$

2 Problem 7.12

If the photon had nonzero mass ($m_\gamma \neq 0$), the Coulomb potential would be replaced by a **Yukawa potential**, of the form

$$V(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0}\frac{e^{-\mu r}}{r} \tag{2.1}$$

where $\mu = \frac{m_\gamma c}{\hbar}$. With a trial wave function of your own devising, estimate the binding energy of a "hydrogen" atom with this potential. Assume $\mu a \ll 1$, and give your answer correct to order $(\mu a)^2$.

Solution:

We know that is ground state of the Hydrogen is given by

$$\psi = \frac{1}{\sqrt{\pi\, a_0^3}}e^{-r/a_0} \tag{2.2}$$

So, let's suppose the "new" hydrogen atom has different Bohr radius, given the new potential. Then Equation 2.2 becomes

$$\psi = \frac{1}{\sqrt{\pi\, b^3}}e^{-r/b} \tag{2.3}$$

where b is the radious parameter we must minimise to find the binding energy of the "hydrogen" atom in the new potential.

Now, let's write our Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{e^{-\mu r}}{r} \tag{2.4}$$

Since our trial wavefunction (Equation 2.4) is already normalised, we can continue to compute $\langle T \rangle$ and $\langle V \rangle$

$$\begin{aligned}
\langle T \rangle &= \frac{1}{\pi\, b^3}\int e^{r/b}\left(\frac{-\hbar^2}{2m}\nabla^2\, e^{-r/b}\right) dr^3 \\
&= -\frac{\hbar^2}{2m\,\pi\, b^3}\int e^{-r/b}\left(\nabla^2\, e^{-r/b}\right) dr^3 \quad \text{(use Equation 1.6)} \\
&= \frac{\hbar^2}{2m\,\pi\, b^4}\int \frac{1}{r^2}\, e^{-2r/b}\left(2r - \frac{r^2}{b}\right) dr^3 \\
&= \frac{\hbar^2}{2m\,\pi\, b^4}\int_0^\infty e^{-2r/b}\left(2r - \frac{r^2}{b}\right) dr\, \underbrace{\int_0^\pi sin\theta d\theta \int_0^{2\pi} d\phi}_{4\pi} \\
&= \frac{4\pi\,\hbar^2}{2m\,\pi\, b^4}\left[2\frac{b^2}{4} - \frac{b^2}{4}\right] = \boxed{\frac{\hbar^2}{2m\, b^2} = \langle T \rangle}
\end{aligned} \tag{2.5}$$

For the integral in Equation 2.5, I used the following formula

$$\int_0^\infty x^n\, e^{-ax} dx = \frac{n!}{a^{n+1}} \tag{2.6}$$

$$\begin{aligned}
\langle V \rangle &= \left(\frac{1}{\pi\, b^3}\right)\left(-\frac{e^2}{4\pi\epsilon_0}\right)\int \frac{1}{r}\, e^{-2r/b}\, e^{-\mu r} dr^3 \\
&= \left(\frac{1}{\pi\, b^3}\right)\left(-\frac{e^2}{4\pi\epsilon_0}\right) 4\pi \int_0^\infty e^{-r(2/b+\mu)}\, r\, dr \\
&= -\frac{e^2}{4\pi\epsilon_0}\frac{4}{b^3}\frac{1}{(2/b+\mu)^2} \\
&= \boxed{-\frac{e^2}{4\pi\epsilon_0}\frac{1}{b\left(1+\frac{\mu\, b}{2}\right)^2} = \langle V \rangle}
\end{aligned} \tag{2.7}$$

Now, use results from Equation 2.5 and Equation 2.7 to define $\langle H \rangle$

$$\langle H \rangle = \frac{\hbar^2}{2m\, b^2} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{b\left(1+\frac{\mu\, b}{2}\right)^2} \tag{2.8}$$

Now, we need to minimise it

$$
\begin{aligned}
\frac{\partial\langle H\rangle}{\partial b} &= -\frac{\hbar^2}{m\,b^3} + \frac{e^2}{4\pi\epsilon_0}\left[\frac{1}{b^2(1+\mu\,b/2)^2} + \frac{\mu}{b\,(1+\mu\,b/2)^3}\right] = 0 \\
0 &= -\frac{\hbar^2}{m\,b^3} + \frac{e^2}{4\pi\epsilon_0}\left[\frac{b(1+\mu b/2)^3 + \mu b^2(1+\mu b/2)^2}{b^3(1+\mu b/2)^5}\right] \\
&= -\frac{\hbar^2}{m\,b^3} + \frac{e^2}{4\pi\epsilon_0}\left[\frac{(1+3\mu b/2)}{b^2(1+\mu b/2)^3}\right] \\
\frac{\hbar^2\,b}{m}\frac{4\pi\epsilon_0}{e^2} &= \frac{(1+3\mu b/2)}{(1+\mu b/2)^3} \\
\frac{\hbar^2}{m}\left(\frac{4\pi\epsilon_0}{e^2}\right) &= b\frac{(1+3\mu b/2)}{(1+\mu b/2)^3} \Rightarrow \boxed{a_0 = b\frac{(1+3\mu b/2)}{(1+\mu b/2)^3}}
\end{aligned}
\tag{2.9}
$$

So, we got a relationship between the Bohr radius, and our new radius. But, there is a cubic relation , then we need to simplify even more using the fact that $\mu a_0 \ll 1$ so we can say that $\mu b \ll 1$ as well.

Using binomial theorem

$$
(1+x)^{-n} = 1 - nx + \frac{n(n+1)}{2!}x^2 + \cdots \tag{2.10}
$$

Therefore

$$
\left(\frac{\mu b}{2}+1\right)^{-3} = 1 - \frac{3\mu b}{2} + \frac{3(\mu b)^2}{2} \tag{2.11}
$$

Now, rewrite Equation 2.9

$$
\begin{aligned}
a_0 &\approx b\left[\left(1+\frac{3\mu b}{2}\right)\left(1-\frac{3\mu b}{2}+\frac{3(\mu b)^2}{2}\right)\right] \\
&\approx b\left(1+\frac{3\mu b}{2}-\frac{3\mu b}{2}-\frac{9(\mu b)^2}{4}+\frac{3(\mu b)^2}{2}+\frac{9(\mu b)^3}{4}\right) \\
&= b\left(1-\frac{3(\mu b)^2}{4}\right) \quad \text{(neglect third order)} \\
b &= \frac{a_0}{\left(1-\frac{3(\mu b)^2}{4}\right)}
\end{aligned}
\tag{2.12}
$$

Expanding in the denominator in the same way, we get

$$
b \approx a_0\left(1+\frac{3(\mu b)^2}{4}\right) \tag{2.13}
$$

Since $\frac{3(\mu b)^2}{4}$ is a really small number, we can write

$$
b \cong a_0\left(1+\frac{3(\mu a_0)^2}{4}\right) \tag{2.14}
$$

Now, replacing this result into Equation 2.8

$$\langle H_{min} \rangle = \frac{\hbar^2}{2m}\frac{1}{a_0^2\left(1+\frac{3(\mu a_0)^2}{4}\right)^2} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{a_0\left(1+\frac{3(\mu a_0)^2}{4}\right)\left(1+\frac{\mu a_0}{2}\right)^2} \tag{2.15}$$

Expanding the denominators

$$\begin{aligned}
\langle H_{min} \rangle &\approx \frac{\hbar^2}{2m\,a_0^2}\left[1-2\frac{3(\mu a_0)^2}{4}\right] - \frac{e^2}{4\pi\epsilon_0\,a_0}\left[1-\frac{3(\mu a_0)^2}{4}\right]\left[1-2\frac{\mu a_0}{2}+3\left(\frac{\mu a_0}{2}\right)^2\right] \\
&= \frac{\hbar^2}{2m\,a_0^2}\left[1-\frac{3(\mu a_0)^2}{2}\right] - \frac{e^2}{4\pi\epsilon_0 a_0}\left[1-\mu a_0+\frac{3(\mu a_0)^2}{4}-\frac{3(\mu a_0)^2}{4}\right] \\
&= -E_1\left[1-\frac{3(\mu a_0)^2}{2}\right] + 2E_1[1-\mu a_0] \\
&= \boxed{E_1\left[1-2\mu a_0+\frac{3}{2}(\mu a_0)^2\right]}
\end{aligned} \tag{2.16}$$

3 Problem 7.13

Suppose you are given a quantum system whose Hamiltonian H_0 admits just two eigenstates, ψ_a (with energy E_a), and ψ_b (with energy E_b). They are orthogonal, normalised , and nondegenerate (assume E_a is the smaller of the two). Now, we turn in a perturbation H', with the following matrix elements:

$$\langle \psi_a | H' | \psi_a \rangle = \langle \psi_b | H' | \psi_b \rangle = 0; \quad \langle \psi_a | H' | \psi_b \rangle = \langle \psi_b | H' | \psi_a \rangle = h \tag{3.1}$$

a) Find the exact eigenvalues of the perturbed Hamiltonian.

b) Estimate the energies of the perturbed system using second-order perturbation theory.

c) Estimate the ground state energy of the perturbed system using variational principle, with a trial function of the form

$$\psi = (cos\phi)\psi_a + (sin\phi)\psi_b \tag{3.2}$$

where ϕ is an adjustable parameter. (Note that writing the linear combination in this way guarantees that ψ is normalised.)

d) Compare your answers to (a), (b), and (c). Why is the variational principle so accurate in this case?

Solution:

a) To find the eigenvalues, we use the following relation

$$\det\left|H-\lambda I\right| = 0 \tag{3.3}$$

But first we need to define H

$$H = H_0 + H' \tag{3.4}$$

Since the eigenstates of the system are orthogonal, and nondegenerate, we can write

$$H_0 = \begin{pmatrix} E_a & 0 \\ 0 & E_b \end{pmatrix} \tag{3.5}$$

and H' is given by the problem as

$$H' = \begin{pmatrix} 0 & h \\ h & 0 \end{pmatrix} \tag{3.6}$$

then, H has the form

$$H' = \begin{pmatrix} E_a & h \\ h & E_b \end{pmatrix} \tag{3.7}$$

Now, let's find the eigenvalues. Using Equation 3.3

$$\begin{aligned} \det \begin{vmatrix} E_a - \lambda & h \\ h & E_b - \lambda \end{vmatrix} &= 0 = (E_a - \lambda)(E_b - \lambda) - h^2 \\ &= E_a E_b - \lambda(E_a + E_b) + \lambda^2 - h^2 \\ \lambda &= \frac{E_a + E_b}{2} \pm \frac{\sqrt{(E_a + E_b)^2 - 4(E_a E_b - h^2)}}{2} \end{aligned} \tag{3.8}$$

Finally

$$\boxed{E_{\pm} = \frac{E_a + E_b}{2} \pm \frac{\sqrt{(E_a - E_b)^2 + 4h^2}}{2}} \tag{3.9}$$

b) Second order perturbation theory is given by

$$E_n = E_n^0 + \langle \psi_n | H' | \psi_n \rangle + \sum_{m \neq n} \frac{\left| \langle \psi_m | H' | \psi_n \rangle \right|^2}{E_n^0 - E_m^0} \tag{3.10}$$

Then, for the given eigenenergies, and using the matrix elements from Equation 3.1

$$\begin{aligned} \tilde{E}_a &= E_a + \frac{\left| \langle \psi_b | H' | \psi_a \rangle \right|^2}{E_a - E_b} \\ &\boxed{E_- = E_a - \frac{h^2}{E_b - E_a}} \end{aligned} \tag{3.11}$$

$$\begin{aligned} \tilde{E}_b &= E_b + \frac{\left| \langle \psi_a | H' | \psi_b \rangle \right|^2}{E_b - E_a} \\ &\boxed{E+ = E_b + \frac{h^2}{E_b - E_a}} \end{aligned} \tag{3.12}$$

c) So, we need to compute $\langle H \rangle$

$$\begin{aligned}
\langle H \rangle &= \langle \psi | H_0 | \psi \rangle + \langle \psi | H' | \psi \rangle \\
&= \langle \cos\phi\, \psi_a + \sin\phi\, \psi_b | H_0 | \cos\phi\, \psi_a + \sin\phi\, \psi_b \rangle \\
&+ \langle \cos\phi\, \psi_a + \sin\phi\, \psi_b | H' | \cos\phi\, \psi_a + \sin\phi\, \psi_b \rangle \\
&= \cos^2\phi\, \langle \psi_a | H_0 | \psi_a \rangle + \sin^2\phi\, \langle \psi_b | H_0 | \psi_b \rangle \\
&+ \sin\phi\, \cos\phi\, \langle \psi_b | H' | \psi_a \rangle + \sin\phi\, \cos\phi\, \langle \psi_a | H' | \psi_b \rangle \\
&= E_a\, \cos^2\phi + E_b\, \sin^2\phi + 2h \sin\phi \cos\phi
\end{aligned} \tag{3.13}$$

Now, we have to minimise $\langle H \rangle$

$$\begin{aligned}
\frac{\partial \langle H \rangle}{\partial \phi} &= -E_a\, 2\cos\phi \sin\phi + E_b\, 2\sin\phi\cos\phi + 2h(\cos^2\phi - \sin^2\phi) \\
0 &= (E_b - E_a)\sin(2\phi) + 2h\cos(2\phi) \\
\tan(2\phi) &= -\frac{2h}{(E_b - E_a)} = -\epsilon, \quad \text{where} \quad \epsilon = \frac{2h}{E_b - E_a}
\end{aligned}$$

we can write ϵ as follows

$$\begin{aligned}
-\epsilon = \frac{\sin(2\phi)}{\sqrt{1 - \sin^2(2\phi)}} &\Rightarrow \sin^2(2\phi) = \epsilon^2(1 - \sin^2(2\phi)) \\
&\Rightarrow \sin^2(2\phi)[1 + \epsilon^2] = \epsilon^2
\end{aligned}$$

Solving for $\sin^2(2\phi)$

$$\sin^2(2\phi) = \frac{\epsilon^2}{1 + \epsilon^2} \Rightarrow \sin(2\phi) = \frac{\pm\epsilon}{\sqrt{1 + \epsilon^2}} \tag{3.14}$$

We can also write

$$\cos^2(2\phi) = 1 - \sin^2(2\phi) = 1 - \frac{\epsilon^2}{1 + \epsilon^2} = \frac{1}{1 + \epsilon^2} \Rightarrow \cos(2\phi) = \frac{\mp 1}{\sqrt{1 + \epsilon^2}} \tag{3.15}$$

the sign is given by $\tan(\phi)$.

But we need to find an expression for $\sin^2\phi$ and $\cos^2\phi$ so we can plug them in our Hamiltonian, therefore i will use the following trig. identities

$$\cos^2\phi = \frac{1}{2}\left(1 + \cos(2\phi)\right) = \frac{1}{2}\left(1 \mp \frac{1}{\sqrt{1 - \epsilon^2}}\right) \tag{3.16}$$

$$\sin^2\phi = \frac{1}{2}\left(1 - \cos(2\phi)\right) = \frac{1}{2}\left(1 \pm \frac{1}{\sqrt{1 + \epsilon^2}}\right) \tag{3.17}$$

taking into account that $2\sin\phi\cos\phi = \sin(2\phi)$, and using the results from 3.14, 3.16, let's rewrite our Hamiltonian

$$\langle H \rangle_{min} = \frac{1}{2}E_a\left(1 \mp \frac{1}{\sqrt{1 + \epsilon^2}}\right) + \frac{1}{2}E_b\left(1 \pm \frac{1}{\sqrt{1 + \epsilon^2}}\right) \pm h\frac{\epsilon}{\sqrt{1 + \epsilon^2}}$$

$$\langle H \rangle_{min} = \frac{1}{2}\left[E_a + E_b \pm \frac{(E_b - E_a + 2h\epsilon)}{\sqrt{1 + \epsilon^2}}\right] \tag{3.18}$$

Simplifying

$$\frac{(E_b - E_a + 2h\epsilon)}{\sqrt{1+\epsilon^2}} = \frac{(E_b - E_a) + 2h\frac{2h}{(E_b-E_a)}}{\sqrt{1+\frac{4h^2}{(E_b-E_a)^2}}}$$
$$= \frac{(E_b - E_a)^2 + 4h^2}{\sqrt{(E_b - E_a)^2 + 4h^2}}$$
$$= \sqrt{(E_b - E_a)^2 + 4h^2} \tag{3.19}$$

So,

$$\langle H \rangle_{min} = \frac{1}{2}\left[E_a + E_b \pm \sqrt{(E_b - E_a)^2 + 4h^2}\right] \tag{3.20}$$

$$\boxed{E_\pm = \frac{1}{2}\left[E_a + E_b \pm \sqrt{(E_b - E_a)^2 + 4h^2}\right]} \tag{3.21}$$

We can see that this result is similar to that obtained in part a (Equation 3.9). Considering that h is very small, we can perform binomial expansion (Equation 2.10)

$$E_\pm = \frac{1}{2}\left[E_a + E_b \pm (E_b - E_a)\sqrt{1 + \frac{4h^2}{(E_b - E_a)^2}}\right]$$

$$E_\pm \approx \frac{1}{2}\left[E_a + E_b \pm (E_b - E_a)\left(1 + \frac{2h^2}{(E_b - E_a)^2}\right)\right]$$

$$E_\pm = \frac{1}{2}\left[E_a + E_b \pm (E_b - E_a) \pm \frac{2h^2}{(E_b - E_a)}\right]$$

Therefore

$$E_- = E_a - \frac{h^2}{(E_b - E_a)} \tag{3.22}$$

$$E_+ = E_b + \frac{h^2}{(E_b - E_a)} \tag{3.23}$$

d) As we can see, results from (c), ((a) follows the same expansion), confirm the perturbation theory results in (b). The variational principle (c) gets the ground state (E_-) exactly right, and this is because the trial wavefunction (Equation 3.2) is almost the most general state.

4 Problem 7.14

As an explicit example of the method developed in Problem 7.13, consider an electron at rest in a uniform magnetic field $\mathbf{B} = B_z\hat{k}$, for which the Hamiltonian is (Equation 4.158)

$$H_0 = \frac{e\,B_z}{m} S_z \tag{4.1}$$

The eigenspinors, χ_a and χ_b, and the corresponding energies, E_a and E_b, are given in Equation 4.161. Now we turn on a perturbation, in the form of a uniform field in the x direction:

$$H' = \frac{e\,B_x}{m} S_x \tag{4.2}$$

a) Find the matrix elements of H', and confirm that they have the structure of Equation 7.55. What is h?

b) Using your result in Problem 7.13 (b), find the new ground-state energy, in second-order perturbation theory.

c) Using your result in Problem 7.13 (c), find the variational principle bound on the ground-state energy.

Solution:

For the electron:

$$\gamma = \frac{-e}{m} \tag{4.3}$$

and, from Equation 4.161, we have that

$$E_{\pm} = \pm \frac{eB_z \hbar}{2m} \tag{4.4}$$

Following the conditions of the Problem 7.13, let $E_a < E_b$, so

$$\chi_a = \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{4.5}$$

$$\chi_b = \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{4.6}$$

$$E_a = E_- = -\frac{eB_z \hbar}{2m} \tag{4.7}$$

$$E_b = E_+ = \frac{eB_z \hbar}{2m} \tag{4.8}$$

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4.9}$$

a)

$$\left\langle \chi_a \middle| H' \middle| \chi_a \right\rangle = \frac{eB_x}{m} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{eB_x \hbar}{2m} \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \tag{4.10}$$

$$\left\langle \chi_b \middle| H' \middle| \chi_b \right\rangle = \frac{eB_x}{m} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \tag{4.11}$$

$$\left\langle \chi_b \middle| H' \middle| \chi_a \right\rangle = \frac{eB_x}{m} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{eB_x \hbar}{2m} \tag{4.12}$$

$$\left\langle \chi_a \middle| H' \middle| \chi_b \right\rangle = \frac{eB_x}{m} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{eB_x \hbar}{2m} \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{eB_x \hbar}{2m} \tag{4.13}$$

Therefore

$$\boxed{h = \frac{eB_x\hbar}{2m}} \tag{4.14}$$

and the conditions of Problem 7.13 are met.

b) From Problem 7.13

$$E_{gs} \approx E_a - \frac{h^2}{(E_b - E_a)} = -\frac{eB_z\hbar}{2m} - \frac{(eB_x\hbar/2m)^2}{eB_z\hbar/m} = \boxed{-\frac{e\hbar}{2m}\left(B_z + \frac{B_x^2}{2B_z}\right)} \tag{4.15}$$

c) From Problem 7.13(c),

$$E_{gs} = \frac{1}{2}\left[E_a + E_b - \sqrt{(E_b - E_a)^2 + 4h^2}\right] \tag{4.16}$$

$$E_{gs} = -\frac{1}{2}\sqrt{\left(\frac{eB_z\hbar}{m}\right)^2 + 4\left(\frac{eB_x\hbar}{2m}\right)^2} = \boxed{-\frac{e\hbar}{2m}\sqrt{B_z^2 + B_x^2}} \tag{4.17}$$

5 Problem 7.17

The fundamental problem in harnessing nuclear fusion is getting the two particles (say, two deuterons) close enough together for the attractive (but short-range) nuclear force to overcome the Coulomb repulsion. The "brute force" method is to heat the particles to fantastic temperatures and allow the random collissions to bring them together. A more exotic proposal is **muon catalysis**, in which we construct a "hydrogen molecule ion", only with deuterons in place of protons, and a (muon) in place of the electron. Predict the equilibrium separation distance between the deuterons in such a structure, and explain why muons are superior to electrons for this purpose.

Solution:

We have to consider the reduced mass concept. Let reduced mass of the muon be m_r, and m_μ be the mass of the muon

$$m_r = \frac{m_\mu m_d}{m_\mu + m_d} = \frac{m_\mu 2m_p}{m_\mu + 2m_p} = \frac{m_\mu}{1 + m_\mu/2m_p}, \quad m_\mu = 207m_e \tag{5.1}$$

$$1 + \frac{m_\mu}{2m_p} = 1 + \frac{207(9.11 \times 10^{-31})}{2(1.67 \times 10^{-27})} = 1.056$$

Therefore

$$m_r = \frac{207\, m_e}{1.056} = 196\, m_e \tag{5.2}$$

, we know that the Bohr radius is defined as

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2\, m_e}$$

but in this case, $m_e \to m_\mu$, therefore, the molecule would shrink by a factor of 196!, bringing the deuterons much closer together, as desired. Thus
For the electron case:

$$R = 2.493\, a_0$$

therefore, for muons:

$$R_\mu = 2.493 \frac{a_0}{196}$$

$$\boxed{R_\mu = 2.493 \frac{0.529 \times 10^{-10}}{196} = 6.73 \times 10^{-13}\, m}$$

We can see that the use of muon, yields to a shorter muonic radious than electronic Bohr radius. This brings the nuclei so close so the strong nuclear force can bind both nuclei together very easily.