PHYS461, Test 1, Spring 2018

You must show work to get credit. There are integrals at the back of the book that might be useful.

In doing variational problems, you might want to re-use trial wave functions (if possible) so you won't have to redo many of the integrals.

(1) (5 pts) Estimate the speed of the electron for the ground state of the hydrogen atom and what will be the fractional change of the ground state energy due to relativity. Clearly give your reasoning. I want numerical values.

(2) (5 pts) Approximate the energy of the ground state of the infinite square well using the trial wave function $\psi_{tr}(x) = Ax(a-x)$. Compare to the exact value and give the percentage your value is above or below the exact value.

(3) (5 pts) An electron is confined between two infinite walls at 0 and a. In addition, there is an extra potential $V(x) = \alpha\delta(x-L)$ where $0 < L < a$. (a) What are the units of alpha? (b) Obtain the eigen-energies, E_n, to order α^2.

(4) (5 pts) As a simple model for a confined atom, treat the case of an electron that interacts with a proton fixed at $r = 0$ and an infinite wall at $r = b$. As accurately as possible find the b where the ground state energy is 0. (Hint: you should first figure out whether perturbation theory or the variational principle is more appropriate.)

(5) (10 pts) A proton is in a potential which is infinite for $x < 0$ and a uniform electric field of $E = 10^5$ V/m pushing it in the negative x direction for $x > 0$. (a) Give the potential energy for the proton. (b) Sketch the potential. (c) Get the ground state energy as accurately as possible. (Make sure to give your answer in J.) (d) Roughly, what is the extent of the wave function. (Make sure to give your answer in meters.)

(6) (10 pts) An atom is in a nearly harmonic well: $V(x) = (1/2)M\omega^2x^2 + Cx^3$. (a) What are the units of C? (b) Obtain the eigen-energies E_n to order C^2.

(7) (10 pts) Two identical particles are confined in an infinite square well $V(x) = 0$ for $0 < x < a$ and is otherwise infinite. There is a small interaction between the two particles which can be approximated as $V(x_1, x_2) = \alpha\delta(x_1 - x_2)$. (a) For $\alpha = 0$, list the energies through $10E_1$ where E_1 is the energy of 1 particle in the infinite square well. (b) Obtain the first 6 eigenenergies to order α^1 and specify any other symmetry that each state has. Write your answer in terms of the symbol $I(n_1, n_2) = \int_0^\pi \sin^2(n_1 x)\sin^2(n_2 x)dx$.

Prob(1)- Roughly the energy scale is $13.6\,eV \simeq 2.2\times10^{-18}\,J$

$$\tfrac{1}{2}mv^2 \sim E \Rightarrow v = \sqrt{\frac{2E}{m}} = \sqrt{\frac{4.4\times10^{-18}\,J}{9.1\times10^{-31}\,kg}} = 2.2\times10^{6}\ m/s$$

Fractional corrections $\sim (v/c)^2 = \left(\frac{2.2\times10^6}{3\times10^8}\right)^2 \sim 5\times10^{-5}$

Prob (2)- First normalize $A^2\int_0^a x^2(a^2-2ax+x^2)\,dx = 1$

$$A^2a^5\left(\tfrac{1}{3}-\tfrac{2}{4}+\tfrac{1}{5}\right) = A^2a^5\left(-\tfrac{1}{6}+\tfrac{1}{5}\right) = \frac{A^2a^5}{30} \Rightarrow A = \sqrt{\frac{30}{a^5}}$$

Now do $\langle KE\rangle = -\frac{\hbar^2}{2m}A^2\int_0^a x(a-x)\left[\frac{d^2}{dx^2}[x(a-x)]\right]dx$

$$= -\frac{\hbar^2}{2m}\frac{30}{a^5}(-2)\int_0^a xa - x^2\,dx = \frac{\hbar^2}{m}\frac{30}{a^5}a^3\left(\tfrac{1}{2}-\tfrac{1}{3}\right)$$

$$= \frac{5\hbar^2}{ma^2} = \frac{\hbar^2}{2ma^2}10$$

The exact value is $\frac{\hbar^2\pi^2}{2ma^2}$

The variational energy is <u>above</u> the exact energy by $(10-\pi^2)/\pi^2 = 0.013$ (1.3%)

Prob(3) - The δ function has units of $\frac{1}{m}$. Units of α are J m

The $E_n^{(0)} = \frac{\hbar^2\pi^2n^2}{2ma^2}$ $\qquad \psi_n^{(0)} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$

$$E_n^{(1)} = \alpha\frac{2}{a}\int_0^a \delta(x-L)\sin^2\left(\frac{n\pi x}{a}\right)dx = \alpha\frac{2}{a}\sin^2\left(\frac{n\pi L}{a}\right) \qquad \text{Eq 6.9}$$

$$E_n^{(2)} = \sum_{m\neq n}\frac{|\langle\psi_m^{(0)}|\alpha\delta(x-L)|\psi_n^{(0)}\rangle|^2}{E_n^{(0)}-E_m^{(0)}} \qquad \text{Eq 6.15}$$

$$= \sum_{m\neq n}\left[E_n^{(0)}-E_m^{(0)}\right]^{-1}\left\{\alpha\frac{2}{a}\sin\left(\frac{n\pi L}{a}\right)\sin\left(\frac{m\pi L}{a}\right)\right\}^2$$

$$= \frac{4\alpha^2}{a^2}\sum_{m\neq n}\frac{\sin^2\left(\frac{n\pi L}{a}\right)\sin^2\left(\frac{m\pi L}{a}\right)}{E_n^{(0)}-E_m^{(0)}}$$

Prob(4) - Use Sec 4.1.3 since this is a spherical potential.
Same as having infinite wall at $r=0$ and $r=b$ and

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{e^2}{4\pi\varepsilon_0 r}$$

Use same trial fct as Prob 2 $\psi_{tr} = Ar(b-r)$

$$\langle KE \rangle = \frac{5\hbar^2}{mb^2}$$

$$\langle PE \rangle = \frac{-e^2}{4\pi\varepsilon_0} A^2 \int_0^b r\,(b^2 - 2br + r^2)\,dr = \frac{e^2}{4\pi\varepsilon_0}\frac{30}{b^5} b^4 \left(\frac{1}{2} - \frac{2}{3} + \frac{1}{4}\right)$$

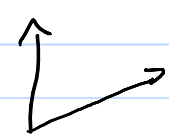
$$= \frac{-e^2}{4\pi\varepsilon_0}\frac{30}{b}\left(-\frac{1}{6} + \frac{1}{4}\right) = -\frac{e^2}{4\pi\varepsilon_0 b}\frac{30}{12} = -\frac{5}{2}\frac{e^2}{4\pi\varepsilon_0 b}$$

The energy is 0 when $\langle KE \rangle + \langle PE \rangle = 0 \Rightarrow \frac{5\hbar^2}{mb^2} = \frac{5}{2}\frac{e^2}{4\pi\varepsilon_0 b}$

$$b = \frac{2\hbar^2}{m}\frac{4\pi\varepsilon_0}{e^2} = 2\,a_0$$ Bohr radius

The actual distance is somewhat smaller because the actual energy is less than $\langle KE \rangle + \langle PE \rangle$

Prob(5) - a) $V = qEx = Fx$ with $F = 1.6\times10^{-14}\,\frac{J}{m}$ b)



c) Any of a number of variational wave fcts are acceptable as long as $\psi(0)=0$ and $\psi(\infty)=0$. Use the one from Prob (2).

$$\langle KE \rangle = \frac{\hbar^2 5}{ma^2}$$

$$\langle PE \rangle = F A^2 \int_0^a x^3(a^2 - 2ax + x^2)\,dx = F\frac{30}{a^5}a^6\left[\frac{1}{4} - \frac{2}{5} + \frac{1}{6}\right]$$

$$= 30Fa\left(-\frac{3}{20} + \frac{1}{6}\right) = \frac{Fa}{2} \Rightarrow E_{tr} = \frac{\hbar^2 5}{ma^2} + \frac{Fa}{2}$$

Find best a $\quad \frac{\partial E}{\partial a} = 0 = -\frac{\hbar^2 10}{ma^3} + F/2 \Rightarrow a = \left(\frac{20\hbar^2}{mF}\right)^{1/3} = 2.03\,\text{nm}$

length scale $\sim a/2 \sim 1\,\text{nm}$

$$E_{tr} = \left(\frac{\hbar^2 F^2}{m}\right)^{1/3}\left[\frac{5}{20^{2/3}} + \left(\frac{20}{8}\right)^{1/3}\right] = 1.19\times10^{-23}\,J \cdot 2.04 = 2.42\times10^{-23}\,J$$

Prob (6) - (a) J/m^3

(b) $E_n^{(0)} = (n+1/2)\hbar\omega$

$$E_n^{(1)} = C\int_{-\infty}^{\infty} \psi_n^2(x)\, x^3\, dx = 0$$

Use Eq 2.69 $x^3 = \left(\frac{\hbar}{2m\omega}\right)^{3/2}(a_+^3 + a_+^2 a_- + a_+ a_- a_+ + a_- a_+^2 + a_-^2 a_+ + a_- a_+ a_- + a_+ a_-^2 + a_-^3)$

The $\langle \psi_n^{(0)} | x^3 | \psi_m^{(0)} \rangle$ are only nonzero for $n = m \pm 3$ and $n = m \pm 1$

$$x^3 \psi_n = \left(\frac{\hbar}{2m\omega}\right)^{3/2}\Big\{\sqrt{(n+1)(n+2)(n+3)}\,\psi_{n+3} + \left[n\sqrt{n+1} + (n+1)\sqrt{n+1} + (n+2)\sqrt{n+1}\right]\psi_{n+1} + \left[(n+1)\sqrt{n} + n\sqrt{n} + (n-1)\sqrt{n}\right]\psi_{n-1} + \sqrt{n(n-1)(n-2)}\,\psi_{n-3}\Big\}$$

$$E_n^{(2)} = \frac{C^2}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^3\Big\{ \underbrace{-\frac{(n+1)(n+2)(n+3)}{3}}_{m=n+3} - \underbrace{\frac{9(n+1)^3}{1}}_{m=n+1} + \underbrace{\frac{9n^3}{1}}_{m=n-1} + \underbrace{\frac{n(n-1)(n-2)}{3}}_{m=n-3} \Big\}$$

Prob (7) - The energies are $E_{n_1,n_2} = E_1 \cdot (n_1^2 + n_2^2)$

a) $\underset{1,1}{2E_1}$, $\underset{1,2}{5E_1}$, $\underset{2,1}{5E_1}$, $\underset{2,2}{8E_1}$, $\underset{1,3}{10E_1}$, $\underset{3,1}{10E_1}$

b) The potential is the same under $x_1 \leftrightarrow x_2$ so do symmetric and antisymmetric combo's

symm
$$E_{1,1}^{(1)} = \frac{4}{a^2}\alpha \int_0^a\int_0^a \delta(x_1-x_2)\sin^2\left(\frac{\pi x_1}{a}\right)\sin^2\left(\frac{\pi x_2}{a}\right)dx_1\,dx_2$$
$$= \frac{4}{a^2}\alpha\int_0^a \sin^4\left(\frac{\pi x}{a}\right)dx = \frac{4\alpha}{\pi a}\, I(1,1)$$

symm
$$E_{1,2+}^{(1)} = \frac{4}{a^2}\alpha\,\frac{1}{2}\int_0^a\int_0^a \delta(x_1-x_2)\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]^2 dx_1\,dx_2$$
$$= \frac{8}{a^2}\alpha\int_0^a \sin^2\left(\frac{\pi x}{a}\right)\sin^2\left(\frac{2\pi x}{a}\right)dx = \frac{8\alpha}{\pi a}\, I(1,2)$$

symm $E_{2,2}^{(1)} = \frac{4\alpha}{\pi a}\, I(2,2)$

symm $E_{1,3+} = \frac{8\alpha}{\pi a}\, I(1,3)$

The antisymmetric functions are 0 at $x_1 = x_2$ so their first order shift is 0.