Solutions to Midterm 2

1. $E = \frac{\hbar^2}{2m} \pi^2 \left(\frac{n_x^2}{L^2} + \frac{n_y^2}{L^2} + \frac{n_z^2}{(10L)^2} \right)$ per neutron

a) ground state: $n_x = n_y = n_z = 1$ for the first 2 neutrons. The 3rd neutron cannot be in the same state since Pauli exclusion principle allow only 1 particle per state (spin allow 2 particles in spatial gnd state)
so 3rd particle has $n_z = 2$

$\therefore E = \frac{\hbar^2}{2m} \pi^2 \left(2 \left(\frac{1+1}{L^2} + \frac{1}{100L^2} \right) + \left(\frac{1+1}{L^2} + \frac{4}{100L^2} \right) \right) = \frac{\hbar^2 \pi^2}{2m} \frac{606}{100L^2}$

b) the 2 neutrons in gnd state have $S=0$ so spin determined by the 3rd neutron

spin $= 1/2$

c) 1st excited state has $n_z = 2$ for a second neutron

$= \frac{\hbar^2 \pi^2}{2m} \frac{609}{100L^2}$

d) There is no degeneracy in spatial state other than wave fn symmetrization. So degeneracy comes from either

having spin 0 and symmetric spatial or
spin 1 and antisymmetric spatial

$\Rightarrow$ degeneracy $= 2$

e) Total spin can be either

$0 \oplus 1/2 = 1/2$ or

$1 \oplus 1/2 = 3/2, \ 1/2$

so spin $= 3/2$ or $1/2$

2\. a) If the 2 electrons are in the same spatial state, spatial wf must be symmetric. Thus, spin must be antisymmetric to satisfy Pauli exclusion principle.

$\Rightarrow$ $S = 0$ only singlet exists

b) electrons in s state are on average closer to the nucleus. Effective charge is therefore larger, since there is less shielding from the 1s electron. Larger effective nuclear charge $\Rightarrow$ lower energy

c) Triplet state has symmetric spin wf $\Rightarrow$ antisymmetric spatial wf. So e on average are further apart than for the singlet. $\therefore$ Coulomb energy of electrons due to each other is smaller for the triplet

$V(x) = \lambda x^4$

3. Variational Method

Find energy for a test wf and vary parameters of the wf to minimize

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \lambda x^4$$

$$\psi = A e^{-\alpha x^2/2}$$

$$\frac{d\psi}{dx} = -\alpha x A e^{-\alpha x^2/2}$$

$$\frac{d^2\psi}{dx^2} = -\alpha A e^{-\alpha x^2/2} + \alpha^2 x^2 A e^{-\alpha x^2/2}$$

$$\therefore H\psi = \frac{-\hbar^2}{2m} A\left(-\alpha + \alpha^2 x^2\right) e^{-\alpha x^2/2} + \lambda^4 x^4 e^{-\alpha x^2/2}$$

$$\langle E \rangle = \frac{\int_{-\infty}^{\infty} \psi^* H \psi \, dx}{\int_{-\infty}^{\infty} \psi^* \psi \, dv} = |A|^2 \int_{-\infty}^{\infty} \left(\left(-\frac{\hbar^2}{2m}\left(-\alpha + \alpha^2 x^2\right) + \lambda^{\cancel{4}} x^4\right) e^{-\alpha x^2} dx \middle/ |A|^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} dx\right.$$

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use the $\int$'s given on the exam:

Since all terms are symmetric about 0
$\int_{-\infty}^{\infty} = 2\int_0^{\infty}$ both in numerator and denominator so choice of limit doesn't matter
(either $\int_0^{\infty}$ or $\int_{-\infty}^{\infty}$ gives same answer)

$$\langle E \rangle = \frac{\left[-\frac{\hbar^2}{2m} \left(-\alpha \, \frac{1}{2} \left(\frac{\pi}{\alpha}\right)^{1/2} + \alpha^2 \frac{1}{4\alpha} \left(\frac{\pi}{\alpha}\right)^{1/2} \right) + \lambda \frac{3}{8\alpha^2} \left(\frac{\pi}{\alpha}\right)^{1/2} \right]}{\frac{1}{2} (\pi/\alpha)^{1/2}}$$

$$\langle E \rangle = -\frac{\hbar^2}{2m} \left(-\alpha + \frac{\alpha}{2} \right) + \frac{3}{4\alpha^2} \lambda$$

$$\frac{d\langle E \rangle}{d\alpha} = -\frac{\hbar^2}{2m} \left(-\frac{1}{2} \right) - \frac{3}{4\alpha^3} (-2) \lambda = 0$$

$$\frac{\hbar^2}{2m} = \frac{3}{2\alpha^3} \lambda$$

$$\alpha^3 = 3\lambda \frac{m}{\hbar^2} \qquad \alpha = \left(3 \frac{\lambda m}{\hbar^2} \right)^{1/3}$$

4. $E(t) = E_0 \, e^{-(t/\tau)^2}$ $\qquad H' = eE(t)x$

if we label our harmonic oscillator states $|n\rangle$ then

$$c_n(t) = \frac{eE}{i\hbar}\int_{-\infty}^{t} dt' \, e^{i\omega_{n0}t'} \langle n|x|0\rangle \, e^{-t'^2/\tau^2}$$

we want the prob at $t=\infty$ so

$$C_n = \frac{eE}{i\hbar}\int_{-\infty}^{\infty} dt' \, e^{i\omega_{n0}t'} \, e^{-t'^2/\tau^2} \langle n|x|0\rangle$$

$$= \frac{eE}{i\hbar}\left[\left(\frac{\pi}{(1/\tau)^2}\right)^{1/2} e^{(i\omega_{n0})^2/2(1/\tau)^2}\right]\langle n|x|0\rangle$$

$$= \sqrt{\pi}\,\frac{eE\tau}{i\hbar} \, e^{\omega_{n0}^2\tau^2/4} \qquad \langle n|x|0\rangle$$

$$P_n = \pi\,\frac{e^2E^2\tau^2}{\hbar^2} \, e^{\omega_{n0}^2\tau^2/4} \qquad |\langle n|x|0\rangle|^2$$

but $\omega_{n0}^2 = \frac{1}{\hbar^2}\left(\hbar\omega(n+\tfrac{1}{2}) - \hbar\omega(\tfrac{1}{2})\right)^2$
$\qquad = n^2\omega^2$

$\langle n|x|0\rangle = 0$ unless $n=1$

using $x = \sqrt{\hbar/2m\omega}\,(A + A^\dagger)$

$$\langle n|x|0\rangle = \frac{\hbar}{2m\omega}\,\delta_{n1}$$

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$$\therefore P_1 = \frac{\pi e^2 E^2 \tau^2}{\hbar^2} e^{n^2 w^2 \tau^2} \frac{\hbar^2}{4m^2 w^2}$$

$$= \frac{\pi e^2 E^2 \tau^2}{4 m^2 w^2} e^{n^2 w^2 \tau}$$