Solution3A.doc

Solution: Quantum Mechanics ~~3A~~ 4A QA

If $\Psi(r)$ is the radial wave function then the equation for $\Phi(r) = r\,\Psi(r)$ can be written as:

$$-\frac{\hbar^2}{2M}\Phi''(r) + \left[V(r) + \frac{l(l+1)\hbar^2}{2Mr^2}\right]\Phi(r) = E\Phi(r),$$

with $\Phi''(r) \equiv \frac{d^2}{dr^2}\Phi(r)$ and $.V(r) = -a\delta(|\vec{r}\,| - \sigma)$

Note: (i) The minimum binding corresponds to $l = 0$
(ii) $\Phi(r=0) = 0$

For $r \neq \sigma$, $V(r) = 0$ and

$$\Phi''(r) - k^2\Phi(r) = 0,$$

where $E < 0$ and $k^2 = \frac{2M\,|E\,|}{\hbar^2}$.

The solutions are obvious:

For $r > \sigma$ $\quad \Phi_>(r) = c_> e^{-kr}$;
For $r < \sigma$ $\quad \Phi_<(r) = c_< \sinh kr$

and satisfy the following two conditions:

(a) $\Phi_>(r=\sigma) = \Phi_>(r=\sigma)$

and, by integrating the radial Schroedinger equation from $\sigma - \varepsilon$ to $\sigma + \varepsilon$, where $\varepsilon \to 0$, :

(b) $-\frac{\hbar^2}{2M}\left[\Phi'_>(\sigma) - \Phi'_<(\sigma)\right] = a\Phi(\sigma)$.

The last equation reduces to:

$$\left[\frac{\Phi'_>(\sigma)}{\Phi_>(\sigma)} - \frac{\Phi'_<(\sigma)}{\Phi_<(\sigma)}\right] = -\alpha = -\frac{2M}{\hbar^2}a \text{ or}$$

$$\coth k\sigma = -1 + \frac{\alpha}{k}$$

The lowest binding energy state will correspond to small $k\sigma$ and thus, in this case, this condition reduces to:

$$\frac{1}{k\sigma} \approx -1 + \frac{\alpha}{k} \quad \text{or} \quad k = \alpha - \frac{1}{\sigma}.$$

Since $k>0$ this implies the final result:

$$a > \frac{\hbar^2}{2M\sigma}$$

CB QM, PS

QA

Consider an electron in the ground state of a tritium atom (H^3). The triton now β-decays to singly ionized Helium-3 (He^{3+}). Assume that both nuclei have infinite mass and that there is no interaction between the β-decay electron and the rest of the system. What is the probability that this new atom will be found in its ground atate?
You may need the following integral:

$$\int_0^\infty u^n e^{-u} du = \Gamma(n+1) \tag{1}$$

where $\Gamma(n+1) = n!$ if n is an integer.

Solution: ~~QA~~ CB

The ground-state wave function ($n = 1, \ell = 0, m = 0$) for a one-electron atom with nuclear charge Ze is:

$$\psi_{100} = Ae^{-\frac{Zr}{a_0}} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Zr}{a_0}} \tag{2}$$

where the constant, A, can be determined by normalizing the integral of the probability density to 1. For the H^3 and He^{3+} ground states we have:

$$\psi_{100}(H^3) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-\frac{r}{a_0}} \tag{3}$$

$$\psi_{100}(He^{3+}) = \frac{1}{\sqrt{\pi}}\left(\frac{2}{a_0}\right)^{3/2} e^{-\frac{2r}{a_0}} \tag{4}$$

And we compute the overlap of initial and final state wave functions to give the probability:

$$\begin{aligned}
\int \psi_{100}(H^3)\psi_{100}(He^{3+})dV &= 4\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{2}{a_0}\right)^{3/2}\int_0^\infty e^{-\frac{3r}{a_0}} r^2 dr && (5)\\
&= \frac{8\sqrt{2}}{a_0^3}\left(\frac{a_0}{3}\right)^3 \int_0^\infty e^{-u}u^2 du && (6)\\
&= \frac{16\sqrt{2}}{27} && (7)\\
&= 0.838 && (8)
\end{aligned}$$

Solution 3B . doc

QC1 QC1

Solution: Quantum Mechanics 3B

Transform Hamiltonians into independent Harmonic oscillator Hamiltonians by simple (canonical) transformations.

(I) $$H_1 = \frac{p^2}{2M} + \frac{1}{2}M\omega^2 x^2 + qEx = \frac{p^2}{2M} + \frac{1}{2}M\omega^2 (x + \frac{qE}{M\omega^2})^2 - \frac{1}{2}\frac{q^2E^2}{M\omega^2}$$

This means that the energy levels are simply shifted harmonic oscillator levels:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{1}{2}\frac{q^2E^2}{M\omega^2}.$$

The ground state wavefunction is then easily obtained as:

$$\Psi(x) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \exp - \left[\frac{M\omega^2\left(x + \frac{qE}{M\omega^2}\right)^2}{2\hbar}\right]$$

(II) $$H_2 = \frac{p_1{}^2}{2M} + \frac{1}{2}M\omega^2 x_1{}^2 + \frac{p_2{}^2}{2M} + \frac{1}{2}M\omega^2 x_2{}^2 + \lambda M\omega^2 (x_2 - x_1)^2.$$

This can be diagonalized by introducing:

$$x_\pm = \frac{1}{\sqrt{2}}(x_1 \pm x_2) \text{ and } p_\pm = \frac{1}{\sqrt{2}}(p_1 \pm p_2) \text{ where } [x_\pm, p_\pm] = i\hbar \text{ and } [x_\pm, p_\mp] = 0$$

By using the obvious identities

$$p_1^2 + p_2^2 = p_+^2 + p_-^2 \text{ and } x_1^2 + x_2^2 = x_+^2 + x_-^2$$

we can rewrite the Hamiltonian as

$$H_2 = \frac{p_+{}^2}{2M} + \frac{1}{2}M\omega^2 x_+{}^2 + \frac{p_-{}^2}{2M} + \frac{1}{2}M\omega'^2 x_-{}^2$$

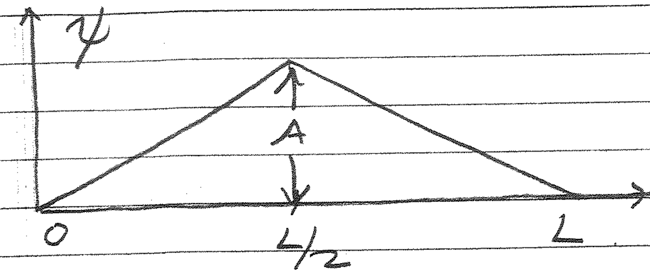
where $\omega' = \sqrt{(1+4\lambda)}\omega$.

The eigenvalues and eigenfunction can then be written by inspection:

$$E(n_+, n_-) = (n_+ + \frac{1}{2})\hbar\omega + (n_- + \frac{1}{2})\hbar\omega'; \quad \Psi_0(x_+, x_-) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4}\left(\frac{M\omega'}{\pi\hbar}\right)^{1/4} e^{-\frac{M\omega^2}{2\hbar}x_+^2} e^{-\frac{M\omega'^2}{2\hbar}x_-^2}$$

QC2 QC2

SOLUTIONS TO PhD EXAM
PROBLEM QM.



$$\psi(x) = x\frac{A}{L/2} = \frac{2xA}{L}, \quad x < L/2$$

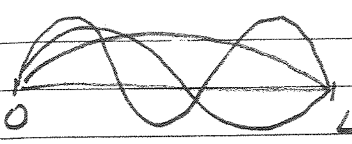
$$\psi(x) = -x\frac{A}{L/2} + B \qquad y(x=L)=0 \qquad B = LA/L/2 = 2A$$

$$= A\left(2 - \frac{2x}{L}\right) = \frac{2A(L-x)}{L}$$

$$\int_0^L \psi^2 dx = 1 = 2\int_0^{L/2}\left(A\frac{2x}{L}\right)^2 dx = \frac{8A^2}{L^2}\int_0^{L/2} x^2 dx$$

$$= \frac{8A^2}{L^2}\frac{1}{3}\left(\frac{L}{2}\right)^3 = \frac{A^2 \cdot L}{3} = 1 \qquad \boxed{A = \sqrt{\frac{3}{L}}}$$

B.



$$\psi = B\sin kx \qquad kx\big|_{x=L} = n\pi$$

$$k = \frac{n\pi}{L} = \frac{2\pi}{\lambda} \qquad n\lambda = 2L \checkmark$$

$$E_n = \frac{p^2}{2m} = \frac{\hbar^2 k_n^2}{2m}$$

$$E_n = n^2\frac{\pi^2\hbar^2}{2mL^2} \qquad \psi = B\sin\frac{n\pi}{L}x \qquad \int_0^L \psi^2 dx = 1 \Rightarrow$$

$$B^2\frac{L}{2} = 1$$

$$B = \sqrt{\frac{2}{L}}$$

C. ψ_n FORM A COMPLETE SET

$$\psi(x) = \sum a_n \sin\frac{n\pi x}{L}$$

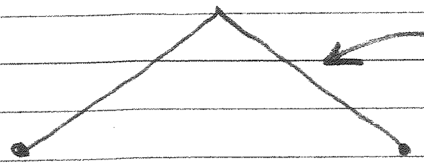
$\times$ by $\sin\frac{m\pi x}{L}$ & INTEGRATE

$$a_n\frac{L}{2} = \int_0^L \psi(x)\sin\frac{n\pi x}{L}dx$$

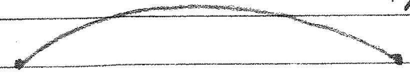
SINCE ψ IS SYMMETRIC ABOUT $x = L/2$

$n = 2, 4, 6, \ldots$ ARE NOT PRESENT

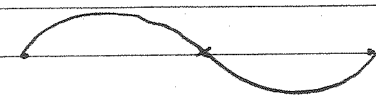
QC2



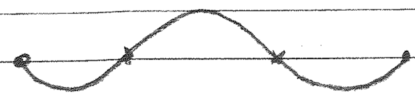
IS A SUM OF $n=1,3,5,..$ MODES ONLY AND HAS NO $n=2,4,6,\ldots$ COMPONENTS



$n=1$

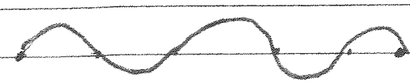


$n=2$



$n=3$

$n=4$



$n=5$

CONTRIBUTE

DON'T CONTRIBUTE THESE ARE ANTI-SYMMETR

$$\frac{L}{2}a_n = 2\int_0^{L/2}\frac{2Ax}{L}\sin\frac{n\pi x}{L}\,dx \qquad y=\frac{n\pi x}{L} \qquad x=\frac{Ly}{n\pi}$$

$$= \frac{4A}{L}\left(\frac{L}{n\pi}\right)^2\int_0^{n\pi/2} y\sin y\,dy \qquad dx=\frac{L\,dy}{n\pi}$$

CHECK ON INTEGRAL.

INTEGRAL $= \sin y - y\cos y$ $\quad \frac{d}{dy}: \cos y - \cos y + y\sin y$

$$\frac{L}{2}a_n = \frac{4A}{L}\left(\frac{L}{n\pi}\right)^2\left(\sin y - y\cos y\right)\Big|_0^{n\pi/2}$$

$$= \frac{4A}{L}\left(\frac{L}{n\pi}\right)^2 \sin\frac{n\pi}{2}\Big|_{n=1,3,\ldots} \text{ ONLY}$$

$$a_n = \frac{8A}{n^2\pi^2}(-1)^n \qquad n=1,3,5,$$

$$a_n = 0 \qquad n=2,4,6,$$

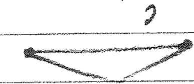
(D) $\psi(t) = \sum a_n \sin\frac{n\pi x}{L}\, e^{iE_nt/\hbar}$ $\qquad E_n = n^2\frac{\hbar^2\pi^2}{2mL^2} = n^2$

REPEATS WHEN $iE_1t/\hbar = 2\pi i$ $\qquad iE_nt/\hbar = 2\pi n^2 i$

$t = T = 2\pi\hbar/E_1$

$t = T/2 \quad iE_1t/\hbar = \pi i \quad e^{\pi i} = -1, \quad e^{iE_nt/\hbar} = e^{in^2\pi}\Big|_{n=1,3,5} = -1$

$\psi(t=T/2) = -\psi(t=0)$



QD1

(c) Configuration is now

$1s^4\, 2s^4\, 2p^5$

$$
\begin{array}{lcccccl}
m_s & \frac{3}{2} & \frac{3}{2} & \frac{3}{2} & \frac{1}{2} & \frac{1}{2} & = \frac{11}{2} \\
m_\ell & 1 & 0 & -1 & 1 & 0 & = \underline{1}
\end{array}
$$

$^{12}P_{9/2}$ ($J = L - S$ since p shell now can hold 12 electrons).

1st inert gas (He analog): $1s^4$, $Z = 4$

2nd " " (Ne analog): $1s^4\, 2s^4\, 2p^{12}$, $Z = 20$

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(3)

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{J^2 - S_1^2 - S_2^2}{2} \quad \text{so}$$

$$H\,|J=1, M\rangle = \frac{4\Delta}{2\hbar^2}\left[J(J+1) - \tfrac{1}{4} - \tfrac{1}{4}\right)|J=1, M\rangle = 3\Delta\,|J=1, M\rangle$$

$$H\,|J=0, M=0\rangle = -\Delta\,|J=1, M=0\rangle$$

where

$$|J=1, M=1\rangle = |\alpha_1 \alpha_2\rangle$$

$$|J=1, M=0\rangle = \frac{1}{\sqrt{2}}\left[|\alpha_1\beta_2\rangle + |\beta_1\alpha_2\rangle\right]$$

$$|J=1, M=-1\rangle = |\beta_1\beta_2\rangle$$

$$|J=0, M=0\rangle = \frac{1}{\sqrt{2}}\left[|\alpha_1\beta_2\rangle - |\beta_1\alpha_2\rangle\right]$$

For $|f\rangle = |\beta_1 \alpha_2\rangle$, $\langle f|H|i\rangle = \frac{3}{2}\Delta + \frac{1}{2}\Delta = 2\Delta$,

$$\omega_{fi} = 0$$

$$c_f = \frac{2\Delta}{i\hbar} \int_0^t dt = \frac{2\Delta t}{i\hbar}$$

$$|c_f(t)|^2 = \frac{4\Delta^2 t^2}{\hbar^2}$$

which disagrees with the exact result for $\frac{4\Delta^2 t^2}{\hbar^2} \gg 1$.

This is because we have not taken into account transitions back into the state $|\alpha_1 \beta_2\rangle$, which become important after sufficient time has elapsed.

~~(4) (a) $\Theta S_i \Theta^{-1} = -S_i$ for any angular momentum operator.~~
~~Then~~

$$\cancel{\Theta S_i^2 \Theta^{-} = \underbrace{\Theta S_i \Theta^{-1}}_{-S_i} \underbrace{\Theta S_i \Theta^{-1}}_{-S_i} = S_i^2 .}$$

~~i.e. H is time reversal invariant.~~

~~(b) Since $S = \frac{3}{2}$, Kramers theorem says that all eigenstates are at least doubly degenerate. We have 4 basis states, $|j, m\rangle$, with $\Theta|j,m\rangle = i^{2j}|j,-m\rangle$~~

~~or~~

QD 1

so $|\alpha_1\beta_2\rangle = \frac{1}{\sqrt{2}}\left[\,|J=1, M=0\rangle + |J=0, M=0\rangle\right]$

$|\beta_1\alpha_2\rangle = \frac{1}{\sqrt{2}}\left[\,|J=1, M=0\rangle - |J=0, M=0\rangle\right]$

(a) $|\Psi(t)\rangle = e^{-iHt/\hbar}\,|\Psi(0)\rangle$

$= \frac{1}{\sqrt{2}}\, e^{-iHt/\hbar}\left[\,|J=1, M=0\rangle + |J=0, M=0\rangle\right]$

$= \frac{1}{\sqrt{2}}\, e^{-3i\Delta t/\hbar}\,|J=1, M=0\rangle + \frac{1}{\sqrt{2}}\, e^{i\Delta t/\hbar}\,|J=0, M=0\rangle$

$\langle\alpha_1\alpha_2|\Psi(t)\rangle = \langle\beta_1\beta_2|\Psi(t)\rangle = 0$

$\langle\alpha_1\beta_2|\Psi(t)\rangle = \frac{1}{2}e^{-3i\Delta t/\hbar} + \frac{1}{2}e^{i\Delta t/\hbar}$

$|\langle\alpha_1\beta_2|\Psi(t)\rangle|^2 = \frac{1}{2}\left[1 + \cos\left(\frac{4\Delta t}{\hbar}\right)\right] \cong 1$ for $\frac{4\Delta t}{\hbar} \ll 1$

and

$|\langle\beta_1\alpha_2|\Psi(t)\rangle|^2 = \frac{1}{2}\left[1 - \cos\left(\frac{4\Delta t}{\hbar}\right)\right] \cong \frac{4\Delta^2 t^2}{\hbar^2}$ for $\frac{4\Delta t}{\hbar} \ll 1$

(b) $i\hbar\,\dot{c}_f = V_{fi}\, e^{i\omega_{fi} t}$, $c_i = 1$ to lowest order.

$\langle\alpha_1\alpha_2|H|\alpha_1\beta_2\rangle = \langle\beta_1\beta_2|H|\alpha_1\beta_2\rangle = 0$, in agreement with above.

~~A similar argument would show that it wont work for electrons in partially filled sub-shells with adjacent values of l.~~
~~A configuration which will work is sd;~~

$$\uparrow \qquad\qquad \uparrow$$
$$m_l = 0 \qquad m_l = 2$$

$S = 1$

$L = 2$

$J = 1$.

~~One might then look to the transition elements, many of which have partially filled s and d shells, but the configurations (more than one subshell) are all of the form~~

$$sd^5, \; sd^4, \; sd^3, \; \text{etc.}$$

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(4) (a) Since $[H, \Theta] = 0$

$\Theta|n\rangle$ is either degenerate with $|n\rangle$ or is (to a phase factor), the same as $|n\rangle$. For spin zero, the latter is the case. Then

$$\Theta|n\rangle = e^{i\delta}|n\rangle,$$ where δ is a constant phase factor.

(b) $\psi_n \equiv \langle \vec{x} | n \rangle$ and under time-reversal,

$\psi_n \to \psi_n^*$ (for the spatial part).

or

$$\langle \vec{x} | \Theta | n \rangle = \langle \vec{x} | n \rangle^* = e^{i\delta} \langle \vec{x} | n \rangle$$

i.e;

$$\psi_n^* = e^{i\delta} \psi_n$$

This implies that ψ_n can always be written as a real function multiplied by a (constant) phase factor. i.e;

For $$\psi_n = e^{-i\delta/2} \Phi_n$$

$$\psi_n^* = e^{i\delta/2} \Phi_n^* = e^{i\delta} e^{-i\delta/2} \Phi_n^*$$

or

$$\Phi_n^* = \Phi_n \quad (\text{real}).$$

(c) Using the completeness of the Y_{lm}'s, the most general form of ψ must be

$$\psi_n = \sum_l \sum_m F_{lm}(r)\, Y_{lm}(\theta, \phi)$$

Now $Y_{\ell m}(\theta,\phi) \propto e^{im\phi}$

and the only <u>real</u> combinations of these are

$$Y_{\ell 0}(\theta,\phi)$$

and $Y_{\ell m} \pm Y_{\ell,-m} \propto \cos m\phi$ or $\sin m\phi$

$\langle L_z \rangle$ in such states is obviously zero.

Since

$$L_x = \frac{1}{2}\left[L_+ + L_-\right]$$

$$L_y = \frac{1}{2i}\left[L_+ - L_-\right]$$

it is also obvious that

$0 = \langle L_x \rangle = \langle L_y \rangle$ for such states.

Yet any combination of such states for a given ℓ yields

$$\langle L^2 \rangle = \ell(\ell+1)\hbar^2.$$

This phenomenon is called "quenching of orbital angular momentum", and occurs when atoms are perturbed by asymmetric external fields, as they will be in a crystal.