Solution: Quantum Mechanics 3A

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

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

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:

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

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

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:

\[ a > \frac{\dot{h}^2}{2M \sigma} \]
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 state?

You may need the following integral:

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

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

**Solution:**

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

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

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:

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

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

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

\[
\int \psi_{100}(H^3)\psi_{100}(He^{3+})dV = 4 \left( \frac{1}{a_0} \right)^{3/2} \left( \frac{2}{a_0} \right)^{3/2} \int_0^\infty e^{-\frac{3r}{a_0}}r^2 dr
\]

\[
= \frac{8\sqrt{2}}{a_0^3} \int_0^\infty e^{-u}u^3 du
\]

\[
= \frac{16\sqrt{2}}{27}
\]

\[
= 0.838
\]
Transform Hamiltonians into independent Harmonic oscillator Hamiltonians by simple (canonical) transformations.

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

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:

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

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

This can be diagonalized by introducing:

\[ x = \frac{1}{\sqrt{2}}(x_1 \pm x_2) \text{ and } p = \frac{1}{\sqrt{2}}(p_1 \pm p_2) \quad \text{where} \quad [x, p] = i\hbar \text{ and } [x, p] = 0 \]

By using the obvious identities

\[ p_1^2 + p_2^2 = p_x^2 + p_y^2 \quad \text{and} \quad x_1^2 + x_2^2 = x_x^2 + x_y^2 \]

we can rewrite the Hamiltonian as

\[ H = \frac{p_x^2}{2M} + \frac{1}{2} M\omega^2 x_x^2 + \frac{p_y^2}{2M} + \frac{1}{2} M\omega^2 x_y^2 \]

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

The eigenvalues and eigenfunction can then be written by inspection:

\[ E(n_+, n_-) = (n_+ + \frac{1}{2})\hbar\omega + (n_- + \frac{1}{2})\hbar\omega' \quad \Psi_0(x_+, x_-) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \left(\frac{M\omega'}{\pi\hbar}\right)^{1/4} e^{-\frac{M\omega^2 x_+^2}{2\hbar}} e^{-\frac{M\omega^2 x_-^2}{2\hbar}} \]
Solutions to PhD Exam

Problem Q.M.

\[ \psi(x) = \begin{cases} \frac{Ax}{L/2}, & x < L/2 \\ \frac{B}{L/2}, & x = L \end{cases} \]

\[ \psi(x) = -x \frac{A}{L/2} + B \quad \psi(x=L) = 0 \quad B = -\frac{LA}{L/2} = 2A \]

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

\[ \int_0^L \psi^2 dx = 1 = 2 \frac{\sqrt{2}}{2} (A^2 x^2) dx = \frac{2A^2}{L} \int_0^{L/2} x^2 dx \]

\[ = \frac{2A^2}{3} \left( \frac{L/2}{3} \right) = \frac{A^2 L}{3} = 1 \quad A = \frac{\sqrt{3}}{L} \]

B.

\[ \psi = B \sin \pi x \quad \psi \bigg|_{x=L} = 0 \]

\[ k = n\pi = \frac{n\pi}{L} \quad n\lambda = 2L \]

\[ E_n = \frac{P^2}{2m} = \frac{k^2}{2m} \]

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

\[ B^2 \frac{L}{2} = 1 \]

\[ B = \sqrt{\frac{2}{L}} \]

C. \( \psi \) forms a complete set

\[ \psi(x) = \sum A_n \sin \frac{n\pi x}{L} \quad x \text{ by } \sin \frac{n\pi x}{L} \]

\[ A_n \frac{1}{2} = \int_0^L \psi(x) \sin \frac{n\pi x}{L} \, dx \]

Since \( \psi \) is symmetric about \( x = L/2 \)

\[ A_n \neq 0 \text{ not present} \]
A sum of \( n = 1, 3, 5, \ldots \) modes only and has no \( n = 2, 4, 6, \ldots \) components.

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\[
\frac{L}{2} q_n = 2 \int_0^{L/2} 2Ax \sin \frac{n \pi x}{L} dx
\]

\[
y = \frac{n \pi x}{L}, \quad x = \frac{L}{n \pi} y
\]

\[
dx = \frac{L}{n \pi} dy
\]

\[
= \frac{4A}{L} \left( \frac{L}{n \pi} \right)^2 \int_0^{n \pi/2} y \sin y dy
\]

\[
\text{CHECK ON INTEGRAL.}
\]

\[
\frac{L}{2} q_n = \frac{4A}{L} \left( \frac{L}{n \pi} \right)^2 (\sin y - y \cos y)
\]

\[
= \frac{4A}{L} \left( \frac{L}{n \pi} \right)^2 \sin \frac{n \pi x}{L}
\]

\[
x = \frac{1}{3}, \frac{5}{3}, \ldots \text{ only}
\]

\[
a_n = \frac{8 \lambda}{n^2 \pi^2}, \quad n = 1, 3, 5, \ldots
\]

\[
a_n = 0, \quad n = 2, 4, 6, \ldots
\]

\[
y(t) = \sum a_n \sin \frac{n \pi x}{L} e^{i \frac{E_n}{M} t}
\]

\[
E_n = \frac{n^2 \pi^2}{2M} = \frac{x^2}{n^2 \pi^2}
\]

Repeats when \( i E_n t/\hbar = 2\pi i \) \( i E_n t/\hbar = 2\pi n^2 i \)

\[
t = T = 2\pi \sqrt{x/\hbar}
\]

\[
t = T/2, \quad i E_n t/\hbar = \pi i, \quad e^{\pi i} = -1, \quad e^{i \pi n^2/\hbar} = (-1)^n
\]

\[
y(t = T/2) = -y(t = 0)
\]
(c) Constitution is now

\[ 1s^2 2s^2 2p^5 \]

\[
\begin{array}{cccccc}
\text{M}_1 & 2 & 2 & 2 & 1 & 1 & \frac{1}{2} \\
\text{M}_2 & 1 & 0 & -1 & 1 & 0 & \frac{1}{2}
\end{array}
\]

\[
\frac{1}{2} = \frac{1}{2}
\]

\[ 2p^{9/2} \quad (J = L = S \text{ since } p \text{ shell now can hold } 12 \text{ electrons}) \]

1st ion gets \((\text{He analogy})\): \[ 1s^2 \quad J = 0 \]

2nd \(\) \((\text{Ne analogy})\): \[ 1s^2 2s^2 2p^{12} \quad J = 20 \]

\[
\frac{s_1 \cdot s_2}{2} = \frac{J^2 - S_1^2 - S_2^2}{2} = 0
\]

\[
H(J = 1, M_J = 4) = \frac{4\alpha}{2\hbar^2} \left[ J(J+1) - \frac{1}{4} - \frac{1}{4} \right] = 3 \alpha \quad (J=1, M_J = 3)
\]

\[
H(J = 0, M_J = 0) = -\alpha \quad (J=1, M_J = 0)
\]

where

\[
\begin{align*}
1J = 1, M_J = 1 & : \{ d_1, d_2 \} \\
1J = 1, M_J = 0 & : \frac{1}{\sqrt{2}} \left[ \left( d_1 \beta_2 \right) + \left( d_2 \beta_1 \right) \right] \\
1J = 1, M_J = -1 & : \left( d_1 \beta_2 \right) \\
1J = 0, M_J = 0 & : \frac{1}{\sqrt{2}} \left[ \left( \omega_1 \beta_2 \right) - \left( \beta_1 d_2 \right) \right]
\end{align*}
\]
For $\mathbf{L} = \mathbf{l}, \mathbf{a}\mathbf{a}$, $\langle \mathbf{L} | \mathbf{H} | \mathbf{L} \rangle = \frac{3}{2} l + \frac{1}{2} a = 2 a,$

$\omega_{da} = 0$

$C_s = \frac{2 \mathbf{a}}{i \hbar} \int_{0}^{t} dt = \frac{-2 \mathbf{a} t}{i \hbar}$

$|C_s(t)|^2 = \frac{4a^2\mathbf{e}^2}{\hbar^2}$

which disagrees with the result due to $\frac{4a^2p^2}{\hbar^2} \approx 1$.

This is because we have not taken into account the transition back into the state $(l_2, p_2)$, which becomes important after sufficient time has elapsed.

(4) (a) $\Theta \mathbf{S}_a \Theta^{-1} = -\mathbf{S}_a$ for any angular momentum $\Theta$.

Then

$\Theta \mathbf{S}_a^2 \Theta^{-1} = \Theta \mathbf{S}_a \Theta^{-1} \Theta \mathbf{S}_a \Theta^{-1} = \mathbf{S}_a^2$.

\[ \Theta \mathbf{S}_a \Theta^{-1} = -\mathbf{S}_a \]

i.e. it is time-reversal invariant.

(b) Since $S = \frac{3}{2}$, Kramer's theorem says only all degenerate states are at least doubly degenerate. We have $N$-basis states, $|l_j, m_j\rangle$ with $\Theta(l, m) = e^{2i \pi l(j - m)}$. 

\[ \Theta \mathbf{S}_a \Theta^{-1} = -\mathbf{S}_a \]
\[
\begin{align*}
\langle \beta_1 \beta_2 | \Psi(t) \rangle &= e^{-\frac{i}{\hbar} H t/\hbar} \langle \beta_1 \beta_2 | \Psi(0) \rangle \\
&= \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar} H t/\hbar} \left[ \langle J=1, M=0 \rangle + \langle J=0, M=0 \rangle \right] \\
&= \frac{1}{\sqrt{2}} e^{-\frac{3}{2} \Delta \omega t/\hbar} \langle J=1, M=0 \rangle + \frac{1}{\sqrt{2}} e^{i \Delta \omega t/\hbar} \langle J=0, M=0 \rangle
\end{align*}
\]

\[
\langle \beta_1 d_2 | \Psi(t) \rangle = \langle \beta_1 \beta_2 | \Psi(t) \rangle = 0
\]

\[
\langle d_1 d_2 | \Psi(t) \rangle = \frac{1}{2} e^{-3 \Delta \omega t/\hbar} + \frac{1}{2} e^{i \Delta \omega t/\hbar}
\]

\[
| \langle \beta_1 d_2 | \Psi(t) \rangle |^2 = \frac{1}{2} \left[ 1 + \alpha \left( \frac{\Delta \omega t}{\hbar} \right) \right] \approx 1 \quad \text{as} \quad \frac{\Delta \omega t}{\hbar} \ll 1
\]

\[
| \langle \beta_1 d_2 | \Psi(t) \rangle |^2 = \frac{1}{2} \left[ 1 - \alpha \left( \frac{\Delta \omega t}{\hbar} \right) \right] \approx \frac{4 \Delta \omega^2 t^2}{\hbar^2} \quad \text{as} \quad \frac{\Delta \omega t}{\hbar} \ll 1
\]

(b) \quad \text{at } t = V_{3,2} e^{i \omega_3 t}, \quad \alpha_3 = 1 \quad \text{to} \quad \text{leave additive}

\[
\langle d_1 d_2 | H | d_1 \beta_2 \rangle = \langle \beta_1 \beta_2 | H | d_1 d_2 \rangle = 0 \quad \text{in agreement with above.}
\]
A similar argument would show that it won't work for electrons in partially filled sub-shells with adjacent values of \( l \). A configuration which will work is \( sdl \):

\[
\begin{align*}
\uparrow & \quad \uparrow \\
 m_c &= 0 & m_b &= 2 \\
 S &= 1 & L &= 2 & J &= 1.
\end{align*}
\]

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

\[
\text{sd}^1, \text{sd}^2, \text{sd}^3, \text{etc.}
\]

(4) (a) Since \( [H_\theta] = 0 \)

\( E(\nu) \) is either degenerate with \( 1m\gamma \) or \( 1 \) (to a phase factor), the same as \( 1m\gamma \). For spin zero, the latter is the case. Then

\[
E(\nu) = e^{i\theta} 1m\gamma, \text{ where } \theta \text{ is a constant phase factor.}
\]
(b) \( \Psi_m = \langle \hat{x} | \Psi \rangle \) and under time-reversal,
\[ \Psi_m \rightarrow \Psi_m^* \quad (\text{with the spatial part}) \]
\[
\langle \hat{x} | \Theta | \Psi \rangle = \langle \hat{x} | \Psi \rangle^* = e^{i\delta} \langle \hat{x} | \Psi \rangle
\]
\[ \text{i.e.} \]
\[ \Psi_m^* = e^{i\delta} \Psi_m \]

This implies that \( \Psi_m \) can always be written as a real function multiplied by a (constant) phase factor. i.e.,
\[ \text{For} \quad \Psi_m = e^{-i\delta/2} \phi_m \]
\[ \Psi_m^* = e^{i\delta/2} \phi_m^* = e^{i\delta} e^{-i\delta/2} \phi_m \]
\[ \phi_m^* = \phi_m \quad \text{(real).} \]

(c) Using the completeness of the \( Y_{lm} \)'s, the most general form of \( \Psi \) must be
\[ \Psi_m = \sum_{l} \sum_{m} \hat{F}_{lm} (\hat{n}) \ Y_{lm} (\theta, \phi) \]
Now \( Y_{lm} (\theta, \phi) \propto e^{im\phi} \)

and the only real combinations are

\( Y_{l0} (\theta, \phi) \)

and

\( Y_{l\pm m} \propto \cos m\phi \) or \( \sin m\phi \)

\( \langle L^2 \rangle \) 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

\[
0 = \langle L_x \rangle = \langle L_y \rangle \text{ for such states.}
\]

Any and combination of states for a given \( l \)

yields

\[
\langle L^2 \rangle = l(l+1) \hbar^2.
\]

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.