Solution QM -A:

(a) Atomic configuration of Eu: $1s^2 2s^2 2p^6 3s^2 2p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^7$.

(b) The 5*d* level has l = 3 and s = ½. We have, therefore $j = l \pm s$ which gives j = 5/2 and j = 3/2, so the orbital spits into two levels $5d^{5/2}$ and $5d^{3/2}$. Each level can accommodate 2*j* + 1 electrons, so there are 6 electrons in the $5d^{5/2}$ level and 4 electrons in the $5d^{3/2}$ level.

(c) For Eu^{3+}, we consider the total spin and total angular momentum of the electrons, so S = 3, L = 3, so $J = |L - S| = 0$ (less than half-filled). Thus, Eu^{3+} is expected to have a moment of 0 μ_B. For Tb^{3+}, S = 3, L = 3, so $J = |L + S| = 6$ (more than half-filled). Thus, Tb^{3+} is expected to have a moment of 12μ_B. (Using $g\sqrt{J(J+1)}\mu_B$, rather than $gJ\mu_B$, should be O.K. too)

SOLUTION QB

Taking into account

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} - \mathbf{F}_0\mathbf{r},$$

we find

$$\frac{d\hat{\mathbf{G}}}{dt} = \frac{\partial\hat{\mathbf{G}}}{\partial t} + \frac{i}{\hbar}[\hat{H}, \hat{\mathbf{G}}] = -\mathbf{F}_0 - \frac{i}{\hbar}[\mathbf{F}_0\mathbf{r}, \hat{\mathbf{p}}] = 0,$$

so that the average

$$\langle\hat{\mathbf{G}}\rangle = \langle\hat{\mathbf{p}}\rangle - \mathbf{F}_0 t = \text{const.}$$

This is a natural quantum mechanical generalization of the statement of classical mechanics that for a particle moving in a uniform field the vector $\mathbf{p}_0 = \mathbf{p}(t) - \mathbf{F}_0 t$ is an integral of motion (since the velocity $\mathbf{v}(t) = \mathbf{v}(0) + \mathbf{F}_0 t/m$) and is equal to particle's momentum at $t = 0$.

Solution QM-C1

2. (a) From the Hamiltonian,

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$$

, where

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial\xi}\right)$$
$$\hat{a}^+ = \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi}\right) \quad \text{and } \xi^2 \equiv \frac{m\omega}{\hbar}x^2 .$$

The ground state can be calculated from the condition, $\hat{a}\varphi_0 = 0$:

$$\varphi_0(x) = Ae^{-\frac{1}{2}\xi^2}$$

For normalization,

$$1 = \int_{-\infty}^{\infty}|\varphi_0|^2 dx = A^2\left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty}e^{-\xi^2}d\xi = A^2\left(\frac{\pi\hbar}{m\omega}\right)^{\frac{1}{2}}$$

Therefore $\varphi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$

(b) When $\omega \rightarrow \frac{1}{2}\omega$, the new ground state is $\varphi^f{}_0 = \left(\frac{m\omega}{2\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{4\hbar}x^2}$

Therefore, the probability that the particle is still in the ground state of the new oscillator is

$$\left\langle \varphi^f{}_0 \middle| \varphi_0 \right\rangle = \left(\frac{1}{2}\right)^{\frac{1}{4}}\left(\frac{4}{3}\right)^{\frac{1}{2}}$$

$$P = \left|\left\langle \varphi^f{}_0 \middle| \varphi_0 \right\rangle\right|^2 = \frac{4}{3\sqrt{2}}$$

Solution QM-C2

(i) The equation of motion for the two-component wave function for $t > 0$ (we have $\jmath = \frac{1}{2}\ \omega$) is,

$$\frac{1}{2} g\mu_B \sigma_x H\psi = i\hbar\partial_t\psi, \tag{1}$$

or

$$\begin{pmatrix} 0 & -i\omega_0 \\ -i\omega_0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \partial_t a \\ \partial_t b \end{pmatrix} \tag{2}$$

where $\omega_0 = g\mu_B\sigma_x H/2\hbar$

We find: $a = \cos\omega_0 t, \quad b = -i\sin\omega_0 t.$

(ii) $\langle J_x\rangle = 0,\ \langle J_y\rangle = -\frac{1}{2}\sin(2\omega_0 t),\ \langle J_z\rangle = \frac{1}{2}\cos(2\omega_0 t).$

(iii) $T > \omega_0^{-1}$.

SOLUTION QM-D1

Recall that operators $\hat{a}$ and $\hat{a}^\dagger$ act in a space of states of the form (here and below summation over n in all equations is from $n = 0$ to $n = \infty$)

$$|\Psi\rangle = \sum c_n |n\rangle = c_0|0\rangle + c_1|1\rangle + \ldots,$$

where $|n\rangle$ stands for the n-particle (quanta) state. Further, recall that

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

Eigenstates $|\alpha\rangle = \sum c_n|n\rangle$ and eigenvalues α of the bosonic annihilation operator $\hat{a}$ are determined by the eigenvalue equation $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$. Since

$$\hat{a}|\alpha\rangle = \sum c_n \sqrt{n}|n-1\rangle = \sum c_{n+1}\sqrt{n+1}|n\rangle,$$

the eigenvalue equation takes the form

$$\sum \left(c_{n+1}\sqrt{n+1} - \alpha c_n \right) |n\rangle = 0.$$

Therefore, taking into account the independence of states $|n\rangle$, we obtain

$$c_{n+1} = \frac{\alpha}{\sqrt{n+1}} c_n = \frac{\alpha}{\sqrt{n+1}} \frac{\alpha}{\sqrt{n}} c_{n-1} = \cdots = \frac{\alpha^{n+1}}{\sqrt{(n+1)!}} c_0.$$

We see that eigenvalues of $\hat{a}$ are arbitrary complex numbers, while the eigenstates can be normalized to one. The normalization condition yields

$$\langle\alpha|\alpha\rangle = \sum_n |c_n|^2 = |c_0|^2 \sum_n \frac{|\alpha|^{2n}}{n!} = 1, \text{ i.e. } |c_0|^2 = e^{-|\alpha|^2}.$$

Thus, the particle number distribution is given by

$$w_n = |c_n|^2 = \exp(-|\alpha|^2) \frac{|\alpha|^{2n}}{n!},$$

which is a Poisson distribution with $\langle n \rangle = |\alpha|^2$.

The eigenvalue problem for the bosonic creation operator $\hat{a}^\dagger|\beta\rangle = \beta|\beta\rangle$ does not have solutions, since the component with the lowest particle number in any state $\beta|\beta\rangle$ is absent in $\hat{a}^\dagger|\beta\rangle$.

QM – D2,   Solutions

For this spherically symmetric potential, the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

for l = 0 and the specified potential reduces to:

$$-\frac{\hbar^2}{2m}\left(R''(r) + \frac{2}{r}R'(r)\right) - \frac{V_o a}{r}e^{-\frac{r}{a}}R(r) = ER(r)$$

(a) Now, we have the trial wave function and can calculate its derivatives:

$$R(r) = e^{-\frac{\beta}{a}r} \Rightarrow R' = \left(-\tfrac{\beta}{a}\right)e^{-\frac{\beta}{a}r} \Rightarrow R'' = \left(\tfrac{\beta}{a}\right)^2 e^{-\frac{\beta}{a}r}$$

and, integrating by parts we have:

$$\int_0^\infty e^{-\frac{2\beta}{a}r} r^2 dr = \frac{2}{\left(\frac{2\beta}{a}\right)^3} \quad \text{and} \quad \int_0^\infty e^{-\frac{2\beta}{a}r} r dr = \frac{1}{\left(\frac{2\beta}{a}\right)^2} \quad \text{and, by extension,} \quad \int_0^\infty e^{-\frac{(2\beta+1)}{a}r} r dr = \frac{1}{\left(\frac{2\beta+1}{a}\right)^2}$$

To employ the variational principle, we wish to find $E(\beta) = \dfrac{\langle R|H|R\rangle}{\langle R|R\rangle}$ (Note: angular integrals cancel.) Writing $\langle R|R\rangle E(\beta) = \langle R|H|R\rangle$ we have

$$\left[\int_0^\infty e^{-\frac{2\beta}{a}r} r^2 dr\right]E(\beta) = -\frac{\hbar^2}{2m}\left[\left(\tfrac{\beta}{a}\right)^2\int_0^\infty e^{-\frac{2\beta}{a}r} r^2 dr + 2\left(-\tfrac{\beta}{a}\right)\int_0^\infty e^{-\frac{2\beta}{a}r} r dr\right] - V_o a\int_0^\infty e^{-\frac{2\beta+1}{a}r} r dr$$

Which reduces to:

$$\left[\frac{2}{\left(\frac{2\beta}{a}\right)^3}\right]E(\beta) = -\frac{\hbar^2}{2m}\left[\left(\tfrac{\beta}{a}\right)^2\frac{2}{\left(\frac{2\beta}{a}\right)^3} - 2\left(\tfrac{\beta}{a}\right)\frac{1}{\left(\frac{2\beta}{a}\right)^2}\right] - V_o a\frac{1}{\left(\frac{2\beta+1}{a}\right)^2}$$

$$= -\frac{\hbar^2}{2m}\left[\left(\tfrac{2}{8}\right)\frac{\left(\frac{\beta}{a}\right)^2}{\left(\frac{\beta}{a}\right)^3} - \left(\tfrac{2}{4}\right)\frac{\left(\frac{\beta}{a}\right)}{\left(\frac{\beta}{a}\right)^2}\right] - \frac{V_o a^3}{(2\beta+1)^2}$$

$$E(\beta) = \left[\frac{\hbar^2}{2m}\frac{1}{4}\frac{a}{\beta} - \frac{V_o a^3}{(2\beta+1)^2}\right]\left[\frac{4\beta^3}{a^3}\right] = \left[\frac{\hbar^2}{2m}\frac{\beta^2}{a^2} - \frac{4V_o\beta^3}{(2\beta+1)^2}\right]$$

(b) For a bound state, must have E < 0 → Find condition for $E(\beta)$ = 0. From above expression for $E(\beta)$, and seeking a solution for β > 0, we see that $E(\beta)$ = 0 when:

$\frac{\hbar^2}{2ma^2} = \frac{4V_o\beta}{(2\beta+1)^2}$ or, equivalently, $\frac{\hbar^2}{8mV_o a^2}(2\beta+1)^2 = \beta$. Rewrite this as $A(2\beta+1)^2 = \beta$ where $A = \frac{\hbar^2}{8mV_o a^2}$. This gives the quadratic equation:

$4\beta^2 + 4\beta + 1 = \frac{\beta}{A} \Rightarrow 4\beta^2 + (4-\frac{1}{A})\beta + 1 = 0$. Find the roots of this quadratic:

$\beta = \frac{-(4-\frac{1}{A}) \pm \sqrt{(4-\frac{1}{A})^2 - 16}}{8}$ for real solutions, need $(4-\frac{1}{A})^2 - 16 > 0$ so

$$\pm(4-\tfrac{1}{A}) - 4 \geq 0 \Rightarrow -4 + \tfrac{1}{A} \geq 4 \Rightarrow \tfrac{1}{A} \geq 8 \Rightarrow A = \frac{\hbar^2}{8mV_o a^2} \leq \tfrac{1}{8} \Rightarrow Vo \geq \frac{\hbar^2}{ma^2}$$

(c) Minimum of energy for this trial wave function is given for β which solves:

$\frac{\partial E(\beta)}{\partial \beta} = 0$ → $\left[\frac{\hbar^2\beta}{ma^2} - \frac{12V_o\beta^2}{(2\beta+1)^2} + \frac{8V_o\beta^3 \cdot 2}{(2\beta+1)^3}\right] = 0$ which, for $\beta \neq 0$ requires solving:

$$\frac{\hbar^2(2\beta+1)^3}{ma^2} - 12V_o\beta(2\beta+1) + 16V_o\beta^2 = 0$$