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Solution for final exam in: FYS3110 - Quantum mechanics.

Date: December 6, 2010 (4 hours).

Problem 1:

1.1 $H = -g\left(|2\rangle\langle 1| + |3\rangle\langle 2| + |1\rangle\langle 3| + |1\rangle\langle 2| + |2\rangle\langle 3| + |3\rangle\langle 1|\right)$ Using the basis $|1\rangle" = "\left(\begin{smallmatrix}1\\0\\0\end{smallmatrix}\right)$, $|2\rangle" = "\left(\begin{smallmatrix}0\\1\\0\end{smallmatrix}\right)$, $|3\rangle" = "\left(\begin{smallmatrix}0\\0\\1\end{smallmatrix}\right)$ we get

$$\underline{H\ " = "\begin{pmatrix}0 & -g & -g\\ -g & 0 & -g\\ -g & -g & 0\end{pmatrix}}$$

1.2 $R = |2\rangle\langle 1| + |3\rangle\langle 2| + |1\rangle\langle 3|$. $R^\dagger = |1\rangle\langle 2| + |2\rangle\langle 3| + |3\rangle\langle 1| \neq R$. R is not Hermitean. $RR^\dagger = |1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3| = I$, so $R^\dagger = R^{-1}$, which implies R is unitary. If R commutes with the Hamiltonian, it represents a symmetry-transformation. Observe that $H = -g\left(R + R^\dagger\right)$.

$$[H, R] = -g\left[R + R^\dagger, R\right] = -g\left(R^\dagger R - RR^\dagger\right) = -g\left(I - I\right) = 0.$$

so R is a symmetry transformation. R corresponds to a rotation by 120 degrees.

1.3 Because R is a rotation by 120 degrees it follows that applying it three times equals the identity operator, thus $R^3 = I$, which also can be checked explicitly. For an eigenstate $|\psi\rangle$

$$I|\psi\rangle = R^3|\psi\rangle = R^2\lambda|\psi\rangle = R\lambda^2|\psi\rangle = \lambda^3|\psi\rangle \tag{1}$$

This means that the eigenvalues λ satisfy $\lambda^3 = 1 \implies \lambda = e^{i2\pi n/3}$ where n is an integer (R is not Hermitean, so complex eigenvalues are allowed). This gives the distinct eigenvalues $\underline{\lambda_1 = 1}$, $\underline{\lambda_2 = e^{i2\pi/3} = -\frac{1}{2} + i\frac{\sqrt{3}}{2}}$ and $\underline{\lambda_3 = e^{-i2\pi/3} = -\frac{1}{2} - i\frac{\sqrt{3}}{2}}$. The matrix representation of R is

$$R\ " = "\begin{pmatrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\end{pmatrix}$$

Labelling the eigenvector $|\psi\rangle" = "\begin{pmatrix} a \\ b \\ c \end{pmatrix}$, the eigenvalue equation $R|\psi\rangle = \lambda|\psi\rangle$ becomes

$$c = \lambda a \quad a = \lambda b \quad b = \lambda c$$

For $\lambda_1 = 1$ we get $a = b = c$ which implies

$$|\psi_1\rangle = \frac{1}{\sqrt{3}}\left(|1\rangle + |2\rangle + |3\rangle\right)$$

For $\lambda_2 = e^{i2\pi/3}$ and setting $b = 1$ we get

$$|\psi_2\rangle = \frac{1}{\sqrt{3}}\left(e^{i2\pi/3}|1\rangle + |2\rangle + e^{-i2\pi/3}|3\rangle\right)$$

and for $\lambda_3 = e^{-i2\pi/3}$ and setting $b = 1$ we get

$$|\psi_3\rangle = \frac{1}{\sqrt{3}}\left(e^{-i2\pi/3}|1\rangle + |2\rangle + e^{i2\pi/3}|3\rangle\right)$$

$|\psi_1\rangle$, $|\psi_2\rangle$ and $|\psi_3\rangle$ form an orthonormal set. Since $[H, R] = 0$ these states are also eigenstates of H. To find the eigenvalues of H observe that $R^\dagger R|\psi_i\rangle = R^\dagger\lambda|\psi_i\rangle = \lambda R^\dagger|\psi_i\rangle \implies \hat{I}|\psi_i\rangle = \lambda R^\dagger|\psi_i\rangle \implies R^\dagger|\psi_i\rangle = \lambda_i^{-1}|\psi_i\rangle$. Therefore

$$H|\psi_i\rangle = -g\left(R + R^\dagger\right)|\psi_i\rangle = -g\left(\lambda_i + \lambda_i^{-1}\right)|\psi_i\rangle$$

So the energies are $E_1 = \underline{-2g}$, $E_2 = -g\left(e^{i2\pi/3} + e^{-i2\pi/3}\right) = -g\,2\cos(2\pi/3) = \underline{g}$ and $E_3 = -g\left(e^{-i2\pi/3} + e^{i2\pi/3}\right) = -g\,2\cos(2\pi/3) = \underline{g}$.

1.4 Observe that the state $|2\rangle = \frac{1}{\sqrt{3}}\left(|\psi_1\rangle + |\psi_2\rangle + |\psi_3\rangle\right)$. Therefore the time-dependent state is

$$|\psi(t)\rangle = \frac{1}{\sqrt{3}}\left(e^{i2gt/\hbar}|\psi_1\rangle + e^{-igt/\hbar}|\psi_2\rangle + e^{-igt/\hbar}|\psi_3\rangle\right)$$

The probability of finding the particle on atom 2 is given by

$$\begin{aligned} P_2 &= |\langle 2|\psi(t)\rangle|^2 = \frac{1}{3}|e^{i2gt/\hbar}\langle 2|\psi_1\rangle + e^{-igt/\hbar}\langle 2|\psi_2\rangle + e^{-igt/\hbar}\langle 2|\psi_3\rangle|^2 \\ &= \frac{1}{3}|e^{i2gt/\hbar}\frac{1}{\sqrt{3}} + e^{-igt/\hbar}\frac{1}{\sqrt{3}} + e^{-igt/\hbar}\frac{1}{\sqrt{3}}|^2 = \frac{1}{9}|1 + 2e^{-i3gt/\hbar}|^2 \\ &= \underline{\frac{1}{9}\left(5 + 4\cos(3gt/\hbar)\right)} \end{aligned}$$

Problem 2:

2.1

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2 y^2 + \frac{p_z^2}{2m} + \frac{1}{2}m\omega^2 z^2 = \underline{\hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)}$$

where $n_i = a_i^\dagger a_i$. The lowest energy level is $E_0 = \underline{\frac{3}{2}\hbar\omega}$ and has $\underline{1}$ state $|000\rangle$. The first excited level has energy $E_1 = \underline{\frac{5}{2}\hbar\omega}$ and consists of the states $|100\rangle, |010\rangle, |001\rangle$ thus is $\underline{3}$-fold degenerate. The second excited level has energy $E_2 = \underline{\frac{7}{2}\hbar\omega}$ and consists of the states $|200\rangle, |020\rangle, |002\rangle, |110\rangle, |101\rangle, |011\rangle$, and is $\underline{6}$-fold degenerate.

2.2 $x = \sqrt{\frac{\hbar}{2m\omega}}\left(a_x^\dagger + a_x\right)$, $y = \sqrt{\frac{\hbar}{2m\omega}}\left(a_y^\dagger + a_y\right)$, $p_x = i\sqrt{\frac{\hbar m\omega}{2}}\left(a_x^\dagger - a_x\right)$, $p_y = i\sqrt{\frac{\hbar m\omega}{2}}\left(a_y^\dagger - a_y\right)$, which gives

$$L_z = i\frac{\hbar}{2}\left[\left(a_x^\dagger + a_x\right)\left(a_y^\dagger - a_y\right) - \left(a_y^\dagger + a_y\right)\left(a_x^\dagger - a_x\right)\right] = \underline{i\hbar\left(a_y^\dagger a_x - a_x^\dagger a_y\right)}$$

2.3 The lowest level:

$$H|000\rangle = E_0|000\rangle, \quad L_z|000\rangle = 0, \quad L^2|000\rangle = 0$$

Thus the ground state has $l = 0$ and $m = 0$. For the first excited level we have the states $|100\rangle$, $|010\rangle$ and $|001\rangle$.

$$L^2|100\rangle = 2\hbar^2|100\rangle, \quad L^2|010\rangle = 2\hbar^2|010\rangle, \quad L^2|001\rangle = 2\hbar^2|001\rangle$$

so all these states have $l = 1$.

$$\begin{aligned} L_z|001\rangle &= 0 \\ L_z|100\rangle &= i\hbar|010\rangle \\ L_z|010\rangle &= -i\hbar|100\rangle \end{aligned}$$

Thus $|001\rangle$ is a state with $l = 1$ and $m = 0$. The states $|100\rangle$ and $|010\rangle$ are not eigenstates of L_z, but the linear combinations

$$|l = 1, m = \pm 1\rangle = \frac{1}{\sqrt{2}}\left(|100\rangle \pm i|010\rangle\right)$$

are. Thus in summary

$$\begin{aligned} |000\rangle &\text{ has } l = 0, m = 0 \\ \frac{1}{\sqrt{2}}\left(|100\rangle + i|010\rangle\right) &\text{ has } l = 1, m = 1 \\ |001\rangle &\text{ has } l = 0, m = 0 \\ \frac{1}{\sqrt{2}}\left(|100\rangle - i|010\rangle\right) &\text{ has } l = 1, m = -1 \end{aligned}$$

2.4 Taking spin into account the degeneracy of the first excited level is 6-fold. These states all have $l = 1$ and $s = 1/2$. The perturbation term can be written

$$\begin{aligned} H_{so} &= \beta\vec{L}\cdot\vec{S} = \frac{\beta}{2}\left(J^2 - L^2 - S^2\right) = \frac{\hbar^2\beta}{2}\left(j(j+1) - l(l+1) - s(s+1)\right) \\ &= \frac{\hbar^2\beta}{2}\left(j(j+1) - 2 - \frac{3}{4}\right) \end{aligned}$$

The eigenstates of J^2 and J_z are good states because these operators commute with H_{so} and H, and the operator $aJ^2 + bJ_z$ have distinct eigenvalues for $a \gg b$. Thus the splitting of this 6-fold degenerate level can be found directly by computing the matrix elements $\langle lsjm_j|H_{so}|lsjm_j\rangle$ for all values of j and m_j. As can be seen from the expression for H_{so} these matrix elements depend only on j and not on m_j. Thus the level will be split in two, one for $j = 3/2$ and one for $j = 1/2$. The $j = 3/2$ level will be $\underline{4}$-fold degenerate and have an energy correction

$$E^1_{j=3/2} = \frac{\hbar^2\beta}{2}\left(\frac{3}{2}\cdot\frac{5}{2} - 2 - \frac{3}{4}\right) = \underline{\frac{\hbar^2\beta}{2}}$$

relative to $E_1 = \frac{5}{2}\hbar\omega$. The $j = 1/2$ level will be $\underline{2}$-fold degenerate and have an energy correction

$$E^1_{j=1/2} = \frac{\hbar^2\beta}{2}\left(\frac{1}{2}\cdot\frac{3}{2} - 2 - \frac{3}{4}\right) = \underline{-\hbar^2\beta}$$

relative to $E_1 = \frac{5}{2}\hbar\omega$. Thus the energy splitting is $\frac{3}{2}\hbar^2\beta$. Such a model; a 3D Harmonic oscillator with spin-orbit coupling, is often used as a simple model to explain the "magic" numbers in the shell structure of nuclei. In that case β is negative.

2.5 Without the contact interaction term the ground state is

$$|\psi(1,2)\rangle = \psi_0(x_1, y_1, z_1)\psi_0(x_2, y_2, z_2)\chi_{12}$$

where χ_{12} is the singlet spin combination which ensures the antisymmetry under the interchange of coordinates. $\psi_0(x, y, z)$ is the product of three one-dimensional harmonic oscillator ground state wavefunctions. The energy of this unperturbed state is $E^0_0 = 2 \times \frac{3}{2}\hbar\omega = 3\hbar\omega$.

The ground state is non-degenerate, so in order to evaluate the energy correction we need

$$
\begin{aligned}
E_0^1 &= \langle \psi(1,2)|V_k|\psi(1,2)\rangle \\
&= \int_{-\infty}^{\infty} dx_1 dy_1 dz_1 dx_2 dy_2 dz_2 \psi_0^*(x_1,y_1,z_1)\psi_0^*(x_2,y_2,z_2) V_k \psi_0(x_1,y_1,z_1)\psi_0(x_2,y_2,z_2) \\
&= \alpha \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dz_1 \, |\psi_0(x_1,y_1,z_1)|^4
\end{aligned}
$$

Using $\psi_0(x,y,z) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}y^2} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}z^2}$ we get

$$
\begin{aligned}
E_0^1 &= \alpha \left(\frac{m\omega}{\pi\hbar}\right)^3 \left[\int_{-\infty}^{\infty} dx e^{-\frac{4m\omega}{2\hbar}x^2}\right] \left[\int_{-\infty}^{\infty} dy e^{-\frac{4m\omega}{2\hbar}y^2}\right] \left[\int_{-\infty}^{\infty} dz e^{-\frac{4m\omega}{2\hbar}z^2}\right] \\
&= \alpha \left(\frac{m\omega}{\pi\hbar}\right)^3 \left[\frac{\pi\hbar}{2m\omega}\right]^{3/2} \\
&= \alpha \left(\frac{m\omega}{2\pi\hbar}\right)^{3/2}
\end{aligned}
$$

Thus the total energy correct to first order in α is $\underline{E_0 = 3\hbar\omega + \alpha\left(\frac{m\omega}{2\pi\hbar}\right)^{3/2}}$.