A toy model of the Helium atom

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PROBLEM

Consider a toy model of the Helium atom where the Coulombic interaction potential is replaced with a Hooke's law potential. If the nucleus of the atom is located at $\vec{r} = 0$ and the electrons of mass m have position vectors $\vec{r}_1$ and $\vec{r}_2$, the interaction potential is

$$V(\vec{r}_1, \vec{r}_2) = \frac{1}{2} m\omega^2 (r_1^2 + r_2^2) - \frac{\lambda}{4} m\omega^2 (\vec{r}_1 - \vec{r}_2)^2$$

This model is exactly solvable. Assume $\lambda > 0$.

(a) What constraint must be imposed on λ for the system to be well-behaved? [Hint: It may be useful to consider the center of mass and relative position vectors of the two electrons $\vec{u} = (\vec{r}_1 + \vec{r}_2)/2$ and $\vec{v} = \vec{r}_2 - \vec{r}_2$.]

(b) What are the energy levels of this system when $\lambda = 1/2$?

(c) Taking into account the spin of the electrons, what are the degeneracies of the lowest four energy levels when $= 1/2$?

(d) Suppose the Helium atom is initially in the third excited state. It then undergoes a decay through an electric dipole transition to a lower-energy state. What are the possible energies of the emitted photon?

SOLUTION TO PART A

The Lagrangian of the this "Helium atom" is

$$L = \frac{1}{2} m\dot{\vec{r}}_1^2 + \frac{1}{2} m\dot{\vec{r}}_2^2 - \frac{1}{2} m\omega^2 (r_1^2 + r_2^2) + \frac{\lambda}{4} m\omega^2 (\vec{r}_1 - \vec{r}_2)^2$$

Now we use the new variables $\vec{u}$ and $\vec{v}$, we can express the coordinates and velocities by them:

$$\vec{r}_1 = \frac{1}{2}(2\vec{u} + \vec{v}) \qquad \dot{\vec{r}}_1 = \frac{1}{2}(2\dot{\vec{u}} + \dot{\vec{v}})$$
$$\vec{r}_2 = \frac{1}{2}(2\vec{u} - \vec{v}) \qquad \dot{\vec{r}}_1 = \frac{1}{2}(2\dot{\vec{u}} - \dot{\vec{v}})$$

Use these variables and we get the transformed Lagrangian

$$L = m\dot{\vec{u}}^2 + \frac{1}{4} m\dot{\vec{v}}^2 - m\omega^2 u^2 - \frac{1}{4}(1 - \lambda) m\omega^2 v^2$$

The canoncial momenta of $\vec{u}$ and $\vec{v}$ are given by $\vec{P}_u = \partial L / \partial \dot{\vec{u}}$ and $\vec{P}_v = \partial L / \partial \dot{\vec{v}}$, then by the Legendre transformation we get the Hamiltonian as shown

$$H = \vec{P}_u \cdot \vec{u} + \vec{P}_v \cdot \vec{v} - L = \frac{P_u^2}{4m} + \frac{P_v^2}{m} + m\omega^2 u^2 + \frac{1}{4}(1 - \lambda) m\omega^2 v^2$$

So when $\lambda < 1$ the system is well-behaved (which means bounded states are not banned.)

SOLUTION TO PART B

Redefine the masses and frequencies as follow:

$$m_u = 2m \qquad \omega_u = \omega$$
$$m_v = \frac{1}{2}m \qquad \omega_v = \frac{\omega}{\sqrt{2}}$$

Then the Hamiltonian becomes

$$H = \frac{P_u^2}{2m_u} + \frac{1}{2}m_u\omega_u^2 u^2 + \frac{P_v^2}{2m_v} + \frac{1}{2}m_v\omega_v^2 v^2$$

Obviously this Hamiltonian is two independent 3D harmonic oscillator. The energy levels are

$$E_{n_u,n_v} = \hbar\omega\left(n_u + \frac{3}{2}\right) + \frac{\hbar\omega}{\sqrt{2}}\left(n_v + \frac{3}{2}\right) \qquad (n_u, n_v = 0, 1, 2, 3, \cdots)$$

SOLUTION TO PART C

Lowest 4 energy levels are given by

$$E_{00} = \frac{3}{2}\left(1 + \frac{1}{\sqrt{2}}\right)\hbar\omega$$
$$E_{01} = \frac{1}{2}\left(3 + \frac{5}{\sqrt{2}}\right)\hbar\omega$$
$$E_{10} = \frac{1}{2}\left(5 + \frac{3}{\sqrt{2}}\right)\hbar\omega$$
$$E_{02} = \frac{1}{2}\left(3 + \frac{7}{\sqrt{2}}\right)\hbar\omega$$

Now we discuss about the degeneracy. For a 3D harmonic oscillator, the degeneracy is given by $g_n = (n+1)(n+2)/2$. So for the energy level E_{n_u,n_v}, the degeneracy of the spacial part of the wave function is $g = (n_u+1)(n_u+2)(n_v+1)(n_v+2)/4$. Now we need to consider about the spin part. Not all of the 4 spin states are possible, we need add Fermi statistics for electrons into consideration. The spacial part wave function is given by

$$\psi_{n_u,n_v}(\vec{r}_1, \vec{r}_2) = \psi_{n_u}\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)\psi_{n_v}(\vec{r}_1 - \vec{r}_2)$$

If $\psi_{n_v}(\vec{v})$ is odd function, then the spacial wave function is antisymmetric under particle permutation, which means we need a spin triplet state for spin part wave functio to keep Fermi statistics, and the degeneracy is multiplied by 3. If $\psi_{n_v}(\vec{v})$ is even function, the spacial wave function is symmetric under particle permutation and we need the spin singlet state spin wave function. From the knowledge of harmonic oscillator, when the quantum number is an even number , then wave function is an even function; when the quantum number is odd, then the wave function is also odd. So the total degeneracy of state E_{n_u,n_v} is

$$g_{n_u,n_v} = \begin{cases} \frac{(n_u+1)(n_u+2)(n_v+1)(n_v+2)}{4} & n_v \text{ even} \\ \frac{3(n_u+1)(n_u+2)(n_v+1)(n_v+2)}{4} & n_v \text{ odd} \end{cases}$$

So the degeneracy of the four lowest energy levels are:

$$\begin{aligned} E_{00}:& \quad \text{1-fold degenerate} \\ E_{01}:& \quad \text{9-fold degenerate} \\ E_{10}:& \quad \text{3-fold degenerate} \\ E_{02}:& \quad \text{6-fold degenerate} \end{aligned}$$

SOLUTION TO PART D

The dipole transition means that the electrons will have a transmition process by a perturbation Hamiltonian which has the following form:

$$H' \sim z_1 + z_2 \sim u_z \sim a_{u_z} + a^\dagger_{u_z}$$

in which $a^\dagger_{u_z}$ and a_{u_z} are creation/annilition operators for corresponding Cartesian coordinate. That Hamiltonian leads to the following seletion rule $\Delta n_u = \pm 1,\ \Delta n_v = 0$. If the initial state is E_{02}, then the possible final state is E_{12}, but it has a higher energy, which means electric dipole decay process is banned. So at the dipole level and the first order perturbation level there is no photon emitted.