

Introduction to Physics of Nanoparticles and Nano structures

Part II: Physics of Nanoparticles

Questions on Module 7

1. Consider the electron states in a AlGaAs/AGaAs split gate dot for which within the Effective Mass Approximation (EMA), the one electron wave function for non interacting electrons in the QD is

$$\Psi(\vec{r}, z) = \phi(\vec{r})\xi_i(z),$$

where \vec{r} is the position vector in the plane of the 2DEG (taken to be the x-y plane at the planer interface of AlGaAs/AGaAs) and z-is the coordinate normal to the 2DEG; here $\xi_i(z)$ is the eigen function for the i^{th} bound state (sub band) in the z-direction, and $\phi(\vec{r})$ satisfies the equation,

$$\left[-\frac{\hbar^2}{2m^*} \nabla_r^2 + V_{eff}(\vec{r}) \right] \phi(\vec{r}) = E\phi(\vec{r}),$$

where m^* is the effective mass in the plane of the dot. As a first approximation, the potential is of parabolic form,

$$V_{eff}(\vec{r}) = \frac{1}{2}m^*\omega_x^2x^2 + \frac{1}{2}m^*\omega_y^2y^2,$$

for which the bound states in the dot are the usual harmonic oscillator solutions, with eigenvalues

$$E(n_x, n_y) = \hbar\omega_x(n_x + 1/2) + \hbar\omega_y(n_y + 1/2),$$

where $n_x, n_y = 0, 1, 2, \dots$. For a AlGaAs/AGaAs split gate dot, these eigenvalues can be several meV.

Show that for $\omega_x = \omega_y = \omega_o$, one has degenerate eigen-states (in addition to spin degeneracy) due to radial symmetry of the problem:

$$E_n = (n + 1)\hbar\omega_o,$$

where $n = n_x + n_y = 0, 1, 2, \dots$. The lowest state $n_x = 0 = n_y$ is non degenerate; the next level $n_x = 1, n_y = 0$ and $n_x = 0, n_y = 1$ is doubly degenerate; and so on. In general, the n^{th} level E_n is $(n + 1)$ -fold degenerate. Show that these degeneracies correspond to different angular momentum states sharing the same energy.

2. Consider the same quantum dot described above, in a magnetic field \vec{B} along z-axis, and for simplicity, assume $\omega_x = \omega_y = \omega_o$. In this case, the one electron Hamiltonian is

$$\mathcal{H} = \frac{1}{2m^*} \left(\vec{p} + \frac{e\vec{A}}{c} \right)^2 + \frac{1}{2}m^*\omega_o^2(x^2 + y^2) + \frac{g^*\mu_B}{\hbar} \vec{B} \cdot \vec{S},$$

where, $\vec{B} = \vec{\nabla} \times \vec{A}$, g^* is the effective Landé's g-factor, and $\mu_B = e\hbar/(2m_e)$ is the Bohr magneton.

Now, choosing a gauge, where $\vec{A} = (-B_y/2, B_x/2, 0)$, so that $\vec{B} = \hat{z}B$ show that

$$\frac{1}{2m^*} \left(\vec{p} + \frac{e\vec{A}}{c} \right)^2 = -\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - \frac{ie\hbar B}{2m^*} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) + \frac{1}{4} \frac{e^2 B^2}{2m^*} (x^2 + y^2).$$

Then show that the Hamiltonian can be rewritten as

$$\mathcal{H} = \mathcal{H}_\omega + \frac{1}{2}\omega_c L_z + \frac{g^*\mu_B}{\hbar} B S_z,$$

where,

$$\mathcal{H}_\omega = -\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{1}{2}m^*\omega^2(x^2 + y^2),$$

with $\omega = \sqrt{\omega_o^2 + \omega_c^2}/2$, and $\omega_c = eB/(cm^*)$ (the cyclotron frequency). Thereby show that the energy eigenvalues are,

$$E_{n,m} = (n+1)\hbar\omega + \frac{1}{2}\hbar\omega_c m \pm \frac{g^*\mu_B}{2} B,$$

where, $m = -n, -(n-2), \dots, (n-2), n$, as shown schematically in the figure, showing $E_{n,m}/\hbar\omega_o$ vs. ω_c/ω_o .

3. Consider now a two electron system QD, with the interaction between the electrons are included. The Hamiltonian for the two electron system in the QD in the magnetic field B may be written as

$$\mathcal{H}(1,2) = \mathcal{H}_o(1) + \mathcal{H}_o(2) + V(|\vec{r}_1 - \vec{r}_2|),$$

where $V(r)$ is the inter-electron Coulomb repulsion, and $\mathcal{H}_o(1), \mathcal{H}_o(2)$ are the Hamiltonian of the individual electrons when they are not interacting, given by

$$\mathcal{H}_o(i) = \frac{p_i^2}{2m^*} + \frac{1}{2}m^*\omega^2 r_i^2 + \frac{1}{2}\omega_c L_{z,i} + \frac{g^*\mu_B}{\hbar} B S_{z,i}.$$

The Hamiltonian $\mathcal{H}(1,2)$ is separable if one introduces the Center of Mass (CM) and Relative (RM) coordinates, defined by

$$\begin{aligned} \vec{R} &= (\vec{r}_1 + \vec{r}_2)/2, & \vec{P} &= (\vec{p}_1 + \vec{p}_2)/2, & \dots\dots\dots & \text{(CM)}, \\ \vec{r} &= \vec{r}_1 - \vec{r}_2, & \vec{p} &= \vec{p}_1 - \vec{p}_2, & \dots\dots\dots & \text{(RM)}. \end{aligned}$$

Show that

$$\begin{aligned} \mathcal{H}(1,2) &= \frac{P^2}{2M} + \frac{1}{2}M\omega^2 R^2 + \frac{1}{2}\omega_c L_z^{CM} \\ &+ \frac{p^2}{2m_r} + \frac{1}{2}m_r\omega^2 r^2 + \frac{1}{2}\omega_c L_z^{RM} + V(r) \\ &+ \frac{g^*\mu_B}{\hbar} B S_z, \end{aligned} ,$$

where $M = m_1 + m_2 = 2m^*$ is the total mass, $m_r = m_1 m_2 / (m_1 + m_2) = m^*/2$ is the reduced mass, and $S_z = \sum_i S_{z,i}$, the z-component of the total spin operator for the two electrons. Show that the energy eigenvalues corresponding to the CM system is

$$E_{CM} = (N+1)\hbar\omega + \frac{1}{2}\hbar\omega_c M, \quad M = -N, -(N-2), \dots, (N-2), N,$$

where N and M denote the principal and angular momentum quantum numbers of the CM system.

The eigen-states of the two-particle system requires consideration of the spin as well as the spatial coordinates in order to find the proper antisymmetric state under the exchange of the

two particles. Considering this show that if the Coulomb interaction $V(r)$ is ignored, then the eigenvalues corresponding to the RM system are given by

$$E_{RM}^0 = (n+1)\hbar\omega + \frac{1}{2}\hbar\omega_c m, \quad m = -n, -(n-2), \dots, (n-2), n,$$

If the Coulomb interaction $V(r)$ is approximated by a parabolic potential, then taking $V(r)$ as,

$$V(r) = V_o - \frac{1}{2}m_r\omega_1^2 r^2,$$

where V_o is a constant, show that the total eigenvalue is

$$E_{NM}^{nm} = V_o + (N+1)\hbar\omega + \frac{1}{2}\hbar\omega_c M + (n+1)\hbar(\omega - \omega_1) + \frac{1}{2}\hbar\omega_c m \pm g^* \mu_B B m_S,$$

References:

1. Transport in Nanostructures, David K. Ferry and Stephen M. Goodnick, (Cambridge University Press, Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, Sao Paulo, 1997, paperback edition 1999, reprinted 2001)

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