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Calculation of hyperfine interaction in spherical quantum dot

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ABSTRACT

In this study, we have calculated the unperturbed wavefunctions and energy eigenvalues of the ground and excited states of a spherical quantum dot, $GaAs/Al_xGa_{1-x}As$, by using quantum genetic algorithm and Hartree–Fock Roothaan method. Hyperfine coupling constant and hyperfine energy of 1*s*, 2*p*, 3*d* and 4*f* levels are carried out as a function of dot radius. The results show that the hyperfine constant and hyperfine energy varies rapidly in the strong and medium confining regions as dot radius decreases. It is worth pointing out that dot radius, impurity charge and angular momentum have a strong influence on the hyperfine energy. It is also found that hyperfine energy and hyperfine splitting vary with aluminium concentration ratio *x*.

1. Introduction

In the last decade, the theoretical study of nanostructures has received increasing attention due to their unusual electronic and optical properties in nanoscience and nanotechnology. Electronic and optical properties of nanostructures such as quantum dots (QDs) can be significantly changed by modifying their parameters as well as the number and type of charge carriers. QDs whose electrons are confined in all three dimensions are sometimes referred to as "artificial atoms" because of having similar properties to real atoms like discrete energy levels and shell structures. Therefore, many research groups have investigated the binding energy and electronic structure [1–5], the electric and magnetic field effects [6–9], the optical properties [10–18] and other physical properties [19–24] of one- and two-electrons QDs with various shape, size and geometry.

An understanding of the nature of impurity states in nanostructures is one of the most important problems in semiconductor physics because the presence of impurity can dramatically alter the electronic, optical and spin properties of QDs [25]. Spins of electron and impurity deal with the fine structure and hyperfine structure of energy spectrum, and understanding the spin-dependent fine and hyperfine structure of energy levels is of high importance in Electron Spin Resonance studies and investigation of impurity properties [26]. Thus, recently, there has been a growing interest in the investigation of electron and impurity spin effects. In the framework effective-mass, Li and Xia [27] and Wang et al. [28] investigated the spin–orbit splitting of a hydrogenic donor impurity. Yakar et al. [29] and Khordad et al. [30] studied the effects of spin–orbit coupling and some relativistic correction terms in spherical QD and a quantum wire using the quantum genetic algorithm and Hartree Fock method and the variational procedure within the effective mass approximation. In the presence of magnetic field by using various methods, the Rashba spin orbit interaction effect on the nonlinear optical properties of QDs was investigated by Hassanabadi et al. [31], Kumar Jha et al. [32] and Vaseghi et al. [33]. In very recently, the nonlinear optical properties and the spin–orbit interactions were performed by Sugirtham et al. [34] by using the compact density

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approach. Similarly, Aytekin et al. [35] studied the spin–orbit effects on the optical properties such as optical rectification, the second and the third harmonic generation coefficient and the change in the refractive index by using the density matrix approach.

The spin of an electron in a 10 nm GaAs QD interacts with $\sim 10^5$ impurity spins [36]. If the spin of an electron interacts with impurity spins, this interaction is referred as hyperfine interaction. Although the hyperfine interaction is relatively weak, it may eventually limit spin coherence of localized electron in QDs or shallow impurities [37,38]. At the same time, this interaction between electron and impurity spin leads to the magnetic hyperfine splitting of energy states and hyperfine structure of spectrum lines. Hyperfine energy deal with hyperfine coupling constant A. Ley-Koo and Garcia-Castelan [39] calculated the Fermi-contact term of the confined hydrogen atom by impenetrable potential surface. Varshni [40] computed the Fermi-contact term for 1s ground state of a compressed hydrogen atom placed at the centre of a spherical box. Similarly, Aquino [41] carried out Fermi-contact term, the nuclear magnetic shielding and polarizability of the confined hydrogen atom. In the above mentioned studies, the Fermi-contact term was calculated for only ground state (1s) of the confined hydrogen. Detailed theoretical studies related with hyperfine splitting and hyperfine constant in the confined hydrogen atom are still lacking, especially in higher states. Therefore, studies in this field are still important for both theoretical research and practical applications.

In the present study, we take into account a spherical QD, GaAs/$Al_xGa_{1-x}As$, inside finite potential well. The unperturbed wavefunctions and energy eigenvalues of *1s*, *2p*, *3d* and *4f* levels are calculated by using quantum genetic algorithm (QGA) and Hartree–Fock Roothaan (HFR) method. In addition, the hyperfine coupling constant and hyperfine energy of the ground and excited states are computed as a function of dot radius for four different values of aluminium concentration ratio x. Also, we investigate the effect of impurity charge on the hyperfine energy.

2. Theory

In the effective-mass approximation, we have considered the spherical QD, in which the hydrogenic impurity is at the centre of spherical quantum dot. The unperturbed Hamiltonian of such a system confined by penetrable spherical surface can be written as follows in atomic units (au)

$$H_0 = -\frac{\nabla^2}{2m^*} - \frac{Z}{\varepsilon_r r} + V_C(r), \tag{1}$$

where Z is the proton number of impurity, m^* and ε_r are the effective mass of electron and relativistic permeability of medium respectively. The term $V_C(r)$ is the spherical confining potential well, and it has the following form

$$V_C(r) = \begin{cases} 0, & r < R \\ V_0, & r \geqslant R \end{cases} \tag{2}$$

where R is dot radius and V_0 is the barrier height. In HFR approximation, impurity is taken into account as a point charge, and impurity has proton(s) and neutron(s). Thus, they distribute in a finite space. This structure of impurity can be expressed by multipole magnetic and electric moments. Magnetic dipole moment, which is the lowest multipole orders of the impurity magnetic moment, makes the most important contribution to hyperfine structure. Since hyperfine structure term is relatively small when compared to the magnitude of unperturbed eigenvalue, it can be considered as perturbation term [42]. Thus, the perturbation Hamiltonian is expressed by

$$\boldsymbol{H}' = \boldsymbol{t^1} \cdot \boldsymbol{\mu_I}, \tag{3}$$

where $\boldsymbol{\mu_I}$ shows the magnetic dipole moment operator of the impurity and $\boldsymbol{t^1}$ is the magnetic dipole operator displaying the magnetic field which is produced by electron at the site of impurity, and it is given by [43]

$$\boldsymbol{t^1} = \frac{\alpha^2}{2}\left[2\boldsymbol{L}r^{-3} - g_s\sqrt{10}(\boldsymbol{SC^2})^1 r^{-3} + g_s\frac{8\pi}{3}\boldsymbol{S}\delta(\boldsymbol{r})\right], \tag{4}$$

in which $\boldsymbol{L}$ and $\boldsymbol{S}$ are orbital and spin angular momentum operator of electron, g_s is the electron spin g-factor, α is fine structure constant and $(\boldsymbol{SC^2})^1$ is a tensor product of $\boldsymbol{S}$ and $\boldsymbol{C^2}$ of rank 1. According to first-order perturbation theory, hyperfine energy is defined as follows

$$W_F = \langle IJFM_F|\boldsymbol{H}'|IJFM_F\rangle, \tag{5}$$

where $|IJFM_F\rangle$ presents the wave function of coupled state. Since hyperfine interaction is considered as a perturbation and μ_I is an operator corresponding to maximum component of impurity spin, $M_I = I$ the wavefunction can be written as $|IJFM_F\rangle = |JM_J\rangle|II\rangle$.

Using $\boldsymbol{t^1}$ and $\boldsymbol{\mu_I}$ operators in Eq. (5), the hyperfine energy W_F is rewritten as follows [43]

$$W_F = \frac{1}{2}A[F(F+1) - I(I+1) - J(J+1)], \tag{6}$$