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Laterally coupled circular quantum dots under applied electric field

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ABSTRACT

The optical response of a system of two laterally coupled quantum dots with circular cross-sectional shape is investigated within the effective mass approximation, taking into account the effects of the change in the geometrical configuration, the application of an external static electric field, and the presence of a donor impurity center. The first-order dielectric susceptibility is calculated in order to derive the corresponding light absorption and relative refractive index coefficients. The possibility of tuning these optical properties by means of changes in the quantum dot symmetry and the electric field intensity is particularly discussed.

1. Introduction

Quantum dots (QDs) are quasi-zero-dimensional systems in which quantum confinement effects account for particular electronic and optical properties in these structures that usually extend over regions sizing a few tens of nanometers [1,2].

In the past decades there have been significant advances on experimental and theoretical research in QDs. A particular interest is placed on the issue of controlling the properties of such nanosystems, looking for prospective device applications as QD lasers [3], photodetectors [4], high-speed electro-optical modulators [5], solid state quantum computing [6], and so forth. Investigating on the influence that the geometrical configuration as well as the presence of external probes, such as strain, hydrostatic pressure and electromagnetic fields, exert on the opto-electronic characteristics of those semiconductor nanostructures is of paramount importance in these endeavours.

Quantum dots are direct candidates for obtaining what has been named as *artificial atoms* (see for instance the review article [7]). When the growth conditions allow for the fabrication of several adjacent QDs, it is usual to find the existence of a kind of inter-dot coupling (mostly related with tunneling effect). Under such conditions one can talk about *artificial molecules* [8–11]. These structures have noteworthy advantages over real atom-made molecules. For instance, it is possible to tune the energy spectrum in them by means of changes in the material composition, the geometry of the QDs, the inter-dot distance and by including dopant atoms. Among the distinct configurations the simplest one considers a pair of QD coupled by sharing a single electron. Two structural setups can be found in this case: vertical and lateral (parallel side by side) coupling. In the latter, the inter-dot coupling breaks the rotational symmetry which turns the theoretical investigation somehow more difficult. There are not many previous reports on laterally coupled QDs. We can mention, for example, the Refs. [12–25].

In the case of 2D QDs, different in-plane geometries were studied by Ezaki et al. [26] who considered the electronic properties of circular, elliptic and, triangular QDs by means of exact diagonalization procedures. Publications on this kind of semiconductor systems appear also in a group of recent investigations dealing with electronic and optical properties under distinct geometrical and potential energy configurations [27–34].

Very recently, Corredor and Gutiérrez put forward a study on the single electron states in a system of two 2D laterally coupled InGaAs-based QDs [35]. The effect of inter-dot electron tunneling and the application of a static electric field were taken into account, revealing the possibility of tuning of inter-state transitions. The work reveals the formation of molecular-like states with features resembling a hydrogen molecule.

In this work we are aimed at studying the optical response of a laterally coupled quantum double QD structure with circular cross-section shape. The inclusion of a donor impurity atom is particularly discussed. The system is assumed to be 3D but with a narrow vertical size. We use the effective mass and parabolic band approximations for determining the allowed electron-impurity states as well as the linear response theory for obtaining the frequency-dependent dielectric susceptibility related with inter-state

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energy transitions. From this latter quantity the expressions of the coefficient of light absorption and the coefficient of relative refractive index change are derived. The calculation includes the presence of an external static electric field -applied along the axis that connects the two dot centers- and changes of the systems geometry take place when the inter-dot distance is varied. Besides, the influence of a ionized donor impurity center is also taken into account. Electron energies and wavefunctions result from a process of exact diagonalization of the Hamiltonian matrix that arises from proposing the solutions in the form of an expansion over a complete set of functions. With the information regarding the quantum states, we then present the results for the mentioned optical coefficients as functions of the geometrical setup and the electric field strength. The paper is organized as follows: in Section 2 we give some key elements of the theoretical model employed, Section 3 is devoted to present and discuss the obtained results and Section 4 contains the conclusions of the study.

2. Theoretical model

Fig. 1 shows a generic 2D picture of the laterally coupled QD system under study as well as a schematic representation of the confining potential profile. Essentially, the $V=0$ active region – made of GaAs – is embedded in a $Ga_{1-x}Al_xAs$ ($x=0.3$) host in which there is a finite potential barrier ($V = V_0$). As mentioned, the structure is considered to have a finite and homogeneous vertical extension. However, the vertical thickness would have a value around 2 nm in such a way that there will be only one quantized state for the motion along this direction. This makes that the description of the electron spectrum and the associated of inter-state energy transitions will entirely rely on the analysis of the 2D motion in the (x,y) plane. As depicted, the electric field points towards the negative x-direction.

In order to perform the calculation of the allowed 3D confined quantum states, the whole structure is assumed to be embedded inside a rectangular potential box with infinite potential barriers and size lengths much larger than the interdot distance.

The Hamiltonian of the system, within the framework of the effective mass approximation, is given by:

$$H = H_0 + |e|\,\vec{F}\cdot\vec{r} - \frac{e^2}{\epsilon_r\,|\vec{r}-\vec{r}_0|}, \tag{1}$$

with H_0 given by

$$H_0 = -\frac{\hbar^2}{2\,m^*}\Delta + V(\vec{r}). \tag{2}$$

The quantities $|e|$ and m^* are the absolute value of the electron charge and the electron effective mass, respectively. Δ is the three-dimensional Laplacian operator and $\vec{r} = (x, y, z)$ is the electron vector position. The vector $\vec{r}_0$ indicates the position of the impurity atom measured from the origin. In this case we have chosen a fixed value, $\vec{r}_0 = (x_2, 0, 0)$.

The solution of the 3D Schrödinger-like effective mass equation – with potential energy function $V(x, y, z)$ – in the parabolic approximation of the energy band is proposed in the form [36];

$$\Psi(x, y, z) = \sqrt{\frac{8}{L_x\,L_y\,L_z}}\sum_{m,n} C_{m,n}\sin\left[\frac{m\,\pi}{L_x}\,x + \frac{m\,\pi}{2}\right] \sin\left[\frac{n\,\pi}{L_y}\,y + \frac{n\,\pi}{2}\right]\cos\left[\frac{\pi}{L_z}\,z\right], \tag{3}$$

where $m = 1, 2, \ldots, m_{max}$ and $n = 1, 2, \ldots, n_{max}$. In accordance, the problem of solving the differential equation turns into the one of finding the eigensystem of an infinite Hamiltonian matrix whose dimensions are in practice truncated in accordance with a chosen convergence criterion (in our case, $m_{max} = n_{max} = 200$). We have set $L_x = L_y = 70$ nm and $L_z = 20$ nm in our calculations.

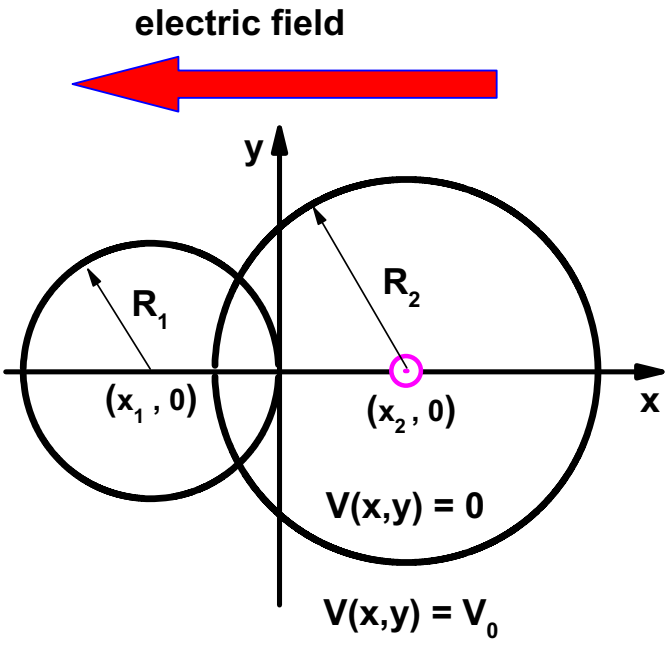

Fig. 1. Pictorial view of the 3D-coupled quantum dot system considered in this work. The center/radius of the two dots are $(x_1, 0)/R_1$ and $(x_2, 0)/R_2$, respectively. The impurity will be always located at the center of the right-hand quantum dot. The system is under applied electric field directed along the negative x-direction. The confinement potential is zero inside the dot regions and V_0 elsewhere. The height of the system, not shown here, is $h=2$ nm.

Restricting ourselves to investigate the linear optical response to an incident electromagnetic radiation of frequency ω, due to transitions between electron-impurity states in the system, the dielectric susceptibility, $\chi^{(1)}(\omega)$, can be obtained within the linear response theory and from its imaginary part we can derive the expression for the light absorption coefficient is given by [37]:

$$\alpha(\omega) = \omega\sqrt{\frac{\mu}{\epsilon_r\,\epsilon_0}}\;\frac{|M_{fi}|^2\,e^2\,\sigma\,\hbar\,\Gamma_{fi}}{(E_{fi}-\hbar\,\omega)^2 + (\hbar\,\Gamma_{fi})^2}; \tag{4}$$

In this expression, the quantity $E_{fi} = E_f - E_i$ is the energy difference associated to the transition between an initial state with energy E_i and a final state E_f. M_{fi} is the electric dipole moment off-diagonal matrix element involving those very states, whereas Γ_{fi} is the corresponding transition damping rate. The quantity ϵ_r is the static dielectric constant, n_r is the refractive index, μ and ϵ_0 are the free space magnetic permeability and dielectric permittivity. Finally, σ is the concentration of carriers participating in the optically-induced transition. In order to determine σ it is necessary to calculate the Fermi level energy, E_F, taking into account that we are assuming them to be at low but nonzero temperature. This implies a self-consistent calculation from the condition

$$n_e = \sum_n \eta_n = 2\sum_n \int_{E_n}^{\infty} dE\; g(E, E_n) f(E, E_F, T), \tag{5}$$

where n_e is the volume density of charge carriers in the conduction band, η_n is the population of the nth energy state, $f(E, E_F, T)$ is the Fermi–Dirac distribution and $g(E, E_n)$ denotes the density of states. In the quantum dot case it is simply written as $\delta(E - E_n)$. Thus, we may write $\sigma = (\eta_i - \eta_f)/V$, where V is the QD volume. Our calculation will assume that in the case of the 3D QDs there will only be two electrons (with oppositely oriented spins) per dot. A system with a finite vertical thickness of 2 nm and the in-plane