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Influence of external field and consequent impurity breathing on excitation profile of doped quantum dots

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ABSTRACT

Excitation in quantum dots is an important phenomenon. Realizing the importance we investigate the excitation behavior of a repulsive impurity doped quantum dot induced by an external oscillatory field. As an obvious consequence the simultaneous oscillation of spatial stretch of impurity domain has also been taken into account. The impurity potential has been assumed to have a Gaussian nature. The ratio of two oscillations (η) has been exploited to understand the nature of excitation. Indeed it has been found that the said ratio could orchestrate the excitation in a truly elegant way. Apart from the ratio, the dopant location also plays some meaningful role towards modulating the excitation rate. The present study also indicates the attainment of stabilization in the excitation rate as soon as η surpasses a threshold value irrespective of the dopant location. Moreover, prior to the onset of stabilization we also envisage minimization in the excitation rate at some typical η values depending on the dopant location. The critical analysis of pertinent impurity parameters provides important perception about the physics behind the excitation process.

1. Introduction

Over the couple of decades we have witnessed an exponential growth in theoretical and experimental researches on impurity states of low-dimensional heterostructures [1,2]. The quantized properties of these doped systems have made them perfect materials for scientific study and technological applications. In view of this, researches on opto-electronic properties of a wide range of semiconductor devices containing impurity have now become worldwide with the excitement of understanding new physics and potential hope for technological impact [3–15].

Miniaturization of semiconductor devices reaches its limit with the advent of quantum dots (QDs). With QD, the subtle interplay between new confinement sources and impurity related potentials has opened up new windows of research in this field [16]. Such confinement, coupled with the dopant location, can dramatically alter the electronic and optical properties of the system [4]. For this reason there are a seemingly large number of theoretical studies on impurity states [17–26]. Added to this, there are also some excellent experimental works which include the mechanism and control of dopant incorporation [27,28].

The emergence of novel experimental and theoretical techniques together with the improvement of traditional ones have made the research on carrier dynamics in nanodevices a ubiquitous one [29,30]. The time-dependent aspects in nanodevices naturally become a hot topic which largely comprises of researches on internal transitions between impurity induced states in a QD [31,32]. These transitions depend on the spatial restriction imposed by the impurity. A minute survey of the dynamical features directs us to explore *excitation* of electrons strongly confined in QD's. Detailed analysis on this aspect deems importance because such excitation provides us with systems for use in opto-electronic devices and as lasers. Within the purview of technological applications such excitation further involves optical encoding, multiplexing, photovoltaic and light emitting devices. The phenomenon also plays some promising role in the eventual population transfer among the exciton states in QD [33,34].

In connection with the dynamical aspects mentioned above there are some important works which study the effect of applied electric field on doped quantum wells and dots [6,35,36]. The aspects discussed above impel us to thoroughly investigate the excitation in doped quantum dots propelled by external oscillatory field. As a result, off late, we have made some investigations on the excitation profiles of the doped quantum dots exposed to oscillatory external field [37]. A deeper physical insight in our problem hitherto outlined reveals some deficiency. The deficiency arises as we have so far considered that the spatial stretch of

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impurity (γ^{-1} in this paper) remains incurious to this external electric field. In practice this spatial stretch depends heavily on magnitude of dot–impurity interaction and any perturbation that affects the said interaction would undoubtedly have tangible influence on the stretch. The energy delivered by an oscillatory external field to the system causes a change in the extent of dot–impurity interaction. And this makes our earlier consideration of uninterrupted impurity spread too stringent to realize. As a result it becomes absolutely essential to assimilate the time-variation of γ in the present study. Of course, this time-dependent alteration in the spatial spread of dopant should not be arbitrary but must be guided by the oscillation frequency of external field. Thus, notwithstanding the tiresome elevation in the mathematical rigor we also incorporate the effect of time-dependent variation of γ in our calculation. We conceive such a *breathing impurity* with a view of making the problem more realistic and reasonable. It needs to be mentioned now that in the present study we have considered that external oscillatory field affects the impurity width only. The other important impurity parameters being impurity location (r_0) and impurity strength (V_0). We felt that it is the impurity width which is most susceptible to a change owing to the external field. V_0 is the inherent strength of impurity potential and is thus expected not to undergo any alteration due to the external field. On the other hand, impurity location may be changed due to the external field but it would require large amount of energy input from the external field. The spatial extension of impurity appears to be the most prominent impurity parameter whose variation due to the external field can be physically realized.

Recently we have done some works on this kind of time-dependent impurity spread in different perspectives [38,39]. Thus, in the present enquiry we have tried to decipher the combined role of oscillatory external field and impurity stretch on the excitation profile. To be precise, in this work we have monitored the ratio of above two oscillation frequencies (termed as *relative oscillation frequency*, ROF and denoted by η where $\nu_1=\eta\nu_2$, ν_1 and ν_2 being the oscillation frequencies of external field and γ, respectively) [38,39] in connection with determining the time-average excitation rate for different dopant locations. Such a response of linear type (i.e. output frequency proportional to input frequency) has been considered for mathematical and computational convenience. Also, such a linear relation can be most easily envisaged and could represent the real situation to some extent. Since the two frequencies are proportional to each other it suggests that there is a kind of linear dependence between them. However, the ratio η simply behaves as a proportionality constant which has been varied arbitrarily in order to monitor the influence of relative strengths of the two frequencies on the excitation kinetics.

A consequent follow up of the dynamics of the doped dot by solving the time-dependent Schrödinger equation containing the time-dependent potential becomes the obvious task to tackle the problem.

2. Method

The model considers an electron subject to a harmonic confinement potential $V(x,y)$ and a perpendicular magnetic field B. The confinement potential assumes the form $V(x,y)=\frac{1}{2}m^*\omega_0^2(x^2+y^2)$, where ω_0 is the harmonic confinement frequency, $\omega_c=eB/m^*c$ being the cyclotron frequency (a measure of magnetic confinement offered by B). In the present work a magnetic field of miliTesla (mT) order has been employed. m^* is the effective electronic mass within the lattice of the material to be used. We have taken $m^*=0.5m_0$ and set $\hbar=e=m_0=a_0=1$. This value of m^* closely resembles *Ge* quantum dots ($m^*=0.55$ a.u.). We have used Landau gauge [$A=(By,0,0)$] where A stands for the vector potential. The Hamiltonian in our problem reads

$$H_0'=-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\frac{1}{2}m^*\omega_0^2x^2+\frac{1}{2}m^*(\omega_0^2+\omega_c^2)y^2-i\hbar\omega_c y\frac{\partial}{\partial x}. \quad (1)$$

Define $\Omega^2=\omega_0^2+\omega_c^2$ as the effective frequency in the y-direction. The model Hamiltonian [cf. Eq. (1)] sensibly represents a 2-d quantum dot with a single carrier electron [40,41]. The form of the confinement potential conforms to a kind of lateral electrostatic confinement (parabolic) of the electrons in the $x-y$ plane [9,17,24,42].

Following earlier works on the effects of a repulsive scatterer in multi-carrier dots in the presence of magnetic field [43,44], here we have considered that the QD is doped with a repulsive Gaussian impurity. Now, as the impurity perturbation is attached to the Hamiltonian [cf. Eq. (1)] it transforms to

$$H_0(x,y,\omega_c,\omega_0)=H_0'(x,y,\omega_c,\omega_0)+V_{imp}(x_0,y_0), \quad (2)$$

where $V_{imp}(x_0,y_0)=V_{imp}(0)=V_0e^{-\gamma_0[(x-x_0)^2+(y-y_0)^2]}$ with $\gamma_0>0$ and $V_0>0$ for repulsive impurity, and (x_0,y_0) denotes the coordinate of the impurity center. V_0 is a measure of the strength of impurity potential whereas γ_0 determines the spatial stretch of the impurity potential. A large value of γ_0 indicates a highly quenched spatial extension of impurity potential whereas a small γ_0 accounts for the spatially dispersed one. Thus, a change in γ_0 in turn causes a change in the extent of dot–impurity overlap that affects the excitation pattern noticeably [37–39]. The parameter γ_0 in the impurity potential is equivalent to $1/d^2$, where d is proportional to the width of the impurity potential [43,44]. The value of γ_0 is taken to be 0.001 a.u. which corresponds to an extension of the impurity domain up to 1.41 nm. The dopant strength (V_0) assumes a maximum value of $\sim10^{-4}$ a.u. or 2.72 meV. The presence of repulsive scatterer simulates dopant with excess electrons. The use of such Gaussian impurity potential is quite well-known [45–47]. In view of the ongoing discussion the work of Gharaati et al. [48] merits mention. They introduced a new confinement potential for the spherical QD's called *modified Gaussian potential, MGP* and showed that this potential can predict the spectral energy and wave functions of a spherical quantum dot.

We write the trial wave function $\psi(x,y)$ as a superposition of the product of harmonic oscillator eigenfunctions $\phi_n(\alpha x)$ and $\phi_m(\beta y)$, respectively, as follows [37–39]:

$$\psi(x,y)=\sum_{n,m}C_{n,m}\phi_n(\alpha x)\phi_m(\beta y), \quad (3)$$

where $C_{n,m}$ are the variational parameters and $\alpha=\sqrt{m^*\omega_0/\hbar}$ and $\beta=\sqrt{m^*\Omega/\hbar}$. In the linear variational calculation, we have used an appreciably large number of basis functions [cf. Eq. (3)] with $n,m=0-20$ for each of the directions (x,y). This direct product basis spans a space of (21×21) dimension. It has been verified that the basis of such size scans the 2-d space effectively completely as long as monitoring the observables under investigation is concerned. A convergence test run by us with still greater number of basis functions confirmed our observation.

The general expressions for the matrix elements of H_0' and V_{imp} are given in Refs. [38,39]. The pth eigenstate of the system in this representation can be written as

$$\psi_p(x,y)=\sum_{ij}C_{ij,p}\{\phi_i(\alpha x)\phi_j(\beta y)\}, \quad (4)$$

where i,j are the appropriate quantum numbers, respectively, and (ij) are composite indices specifying the direct product basis.