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Excitation kinetics of quantum dot induced by damped propagation of dopant: Role of confinement potential and magnetic field

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ABSTRACT

We investigate the excitation kinetics of a repulsive impurity doped quantum dot as the dopant is propagating. The study assumes importance because of its intimate connection with impurity drift in nanodevices. The problem has been made more realistic by considering the dopant propagation to be damped. For simplicity, we have considered an inherently linear motion of the dopant with a Gaussian potential. The damping strength and the dot confinement sources of electric and magnetic origin have been found to fabricate the said kinetics in a delicate way. The present study sheds light on how the individual or combined variation of different confinement sources could design the excitation kinetics in presence of damping. However, in the overdamped region, we find attainment of stabilization in the excitation rate. The present investigation is believed to provide some useful perceptions in the phenomenon of damping that has potential importance in nanoelectronic applications.

1. Introduction

Over the last couple of decades we have noticed a hike in theoretical and experimental researches on impurity states of low-dimensional heterostructures [1]. Out of these heterostructures, quantum dot (QD), beyond any doubt, is one of the most celebrated candidates. Basically, the journey towards miniaturization of semiconductor devices culminates in QD's. The properties of doped QD's have made them potential candidates for scientific study and technological applications. With QD, the subtle interplay between new confinement sources and impurity potentials has opened up new areas of research in this field [2]. Under the confinement, the dopant location manifestly alters the electronic and optical properties of the system [3]. For this reason there is a vast literature comprising of theoretical studies on impurity states [4–13] in general, and also on their opto-electronic properties, in particular, for a wide range of semiconductor devices [3,14–27]. The research trend has become ubiquitous with the excitement of delving into new physics and sincere hope for profound technological impact.

A parallel thrust, however, can also be witnessed in the research on carrier dynamics in nanodevices [28] which largely consists of internal transitions between impurity induced states in QD [29,30]. These transitions depend on the spatial constraints imposed by the impurity. The dynamical aspects propel us explore the *excitation* of electrons strongly confined in QD's. Looking at the possibility of potential usage in opto-electronic devices and as lasers, a scrupulous analysis on excitation kinetics deems real importance. From the perspective of technological applications such excitation further involve optical encoding, multiplexing, photovoltaic and light emitting devices. The phenomenon also plays some important role in the population transfer among the exciton states in QD [31].

Of late, we have investigated the salient features of excitation in doped QD which is induced by a time-dependent propagation of the dopant coordinate [32,33]. Such time-dependent propagation of dopant site bears close correlation with impurity drift in semiconductor nanodevices. The said study has attracted a great deal of interest as most low-dimensional structures contain doped regions. The impurities can be introduced by diffusion [34] and they experience some kind of *force* applied by the dot confinement potential [35]. Sundqvist et al. in their work [36] considered diffusion of ionized impurities interacting with electrons experimentally. In their work the impurity profiles in low-dimensional structures were regulated by an external parabolic potential defined by a variety of gate arrangements and they maintained impurity profiles of typical Gaussian shape. Later on we have further improved our previous theoretical framework [32,33] by incorporating time-dependent alteration in the spatial stretch of the dopant associated with its drift [37].

The problem of *damping* in QD is of immense importance not only for fundamental physics but also for nanoelectronic applications. The manufacture of high quality single electron transistors [38], logic elements (quantum bits) [39], memory

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cells [40], and lasers based on QD heterostructures [41] is intimately related to the damping phenomenon in the system. The phenomenon appears more important since nanoelectronic devices are often introduced into large integral circuits studded with closely packed structural elements [42]. The characteristic length between the elements of integral circuits generally falls within the range of several tens of nanometers. These nanoelectronic devices mutually influence one another and also get affected by the metallic and doped semiconductor fragments of the heterostructures and integrated circuits. It has also been found that impurities are very much related with damping [43–45] and different elementary excitation localized inside a QD interfere with the damping [42]. The QD carriers have been found to be strongly interacting with environmental excitation in the vicinity of dots containing doped components. Consequently, several studies on the QD electronic damping dynamics affected by interactions with the environmental excitation have been performed [39]. There are also some experimental studies to probe damping in doped quantum confined structures by optical techniques [46].

In the present manuscript we have investigated the role of *damping*, coupled with diverse values of confinement potential and magnetic field, on the excitation kinetics of doped QD. The confinement potential in quantum dots plays important role in transport processes and the form of the confinement potential can be experimentally modulated. A variation in magnetic field can help us examine the transitions between the bound states of the dot. Recently, it has also been shown that some typical orientation of magnetic field can tune the binding energy of surface impurities in QD's [47]. It is because of damping the propagation of dopant with respect to fixed dot confinement center will be hindered. For simplicity we have confined ourselves to linear propagation of dopant and the restriction imposed on it has been modeled by introducing an exponentially decaying term into its motion. The parameter ζ inside the exponential takes care of the influence of damping. Following our earlier work [37] we have also considered the appropriate time-dependent modulation of spatial stretch of impurity (γ^{-1}) associated with the damped movement of the dopant. We have determined the time-average excitation rate ($\langle R_{ex}\rangle$) as a function of dot confinement potential (ω_0) and cyclotron frequency (ω_c, a measure of strength of magnetic field) under low, intermediate, and highly damped conditions. To make the study more self-contained we have also explored the combined role of ω_0 and ω_c (also a kind of confinement) on the excitation kinetics in terms of their ratio ($\omega_r = \omega_0/\omega_c$). The study has been further consolidated with the determination of $\langle R_{ex}\rangle$ as a function of damping parameter ζ. The various profiles unveil the subtle roles played by the confinement potential and the magnetic field on the excitation kinetics as the dopant propagation gets damped to different extents.

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, $\omega_c = \frac{eB}{m^*c}$ 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 [48,49]. The form of the confinement potential conforms to kind of lateral electrostatic confinement (parabolic) of the electrons in the $x-y$ plane [4,5,19,27,50].

In the present problem we have considered that the QD is doped with a repulsive Gaussian impurity [51,52]. Introducing the impurity potential 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 $V_{imp}(x_0,y_0) = V_{imp}(0) = V_0\, e^{-\gamma_0\left[(x-x_0)^2+(y-y_0)^2\right]}$ 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^{-1} determines the spatial stretch of the impurity potential. The presence of repulsive scatterer simulates dopant with excess electrons. The use of such Gaussian impurity potential is quite well-known [53–55]. Gharaati et al. [56] 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.

The time-independent Schrödinger equation has been solved using variational method expressing the trial wave function $\psi(x,y)$ as a superposition of the product of harmonic oscillator eigenfunctions [32,33,37,57]. In the linear variational calculation, an appreciably large number of basis functions have been exploited after making the required convergence test.

Now, we introduce the time-dependence into the dopant coordinate so that $x_0 \to x_0(t)$ and $y_0 \to y_0(t)$. However, in keeping with our improved theoretical framework [37], γ also becomes time-dependent as a result of dopant propagation. Such a time-dependent spatial enhancement of dopant potential recognizes the signature of instantaneous location of the dopant on its spatial extension. The time-dependence reads as $\gamma(t) = \gamma_0 \exp\left\{-\eta\sqrt{x_0^2(t)+y_0^2(t)}\right\}$, where η is a very small parameter and γ_0 is the initial value of γ. Thus, it is nothing but an indolent enhancement of the region over which the influence of dopant is disseminated owing to its drift. Now the time-dependent Hamiltonian reads

$$H(t) = \left[H_0 - V_{imp}(0)\right] + V_1(t), \quad (3)$$

where

$$V_1(t) = V_0\, e^{-\gamma(t)\left[\{x-x_0(t)\}^2+\{y-y_0(t)\}^2\right]} \quad (4)$$

In the present paper the time-dependence of dopant propagation has been considered to be linear so that $x_0(t) = x_0 + at, y_0(t) = y_0 + bt$. We now introduce the effect of damping into it phenomenologically through the parameter ζ (a measure of damping strength) giving rise to $x_0(t) = (x_0+at)e^{-\zeta t}$ and $y_0(t) = (y_0+bt)e^{-\zeta t}$. Such representation ensures a quicker fall of dopant propagation with increase in the damping strength in comparison with the undamped motion. The matrix element involving any two arbitrary eigenstates p and q of H_0 due to $V_1(t)$ reads (for details of derivation see [57]).

$$\begin{aligned} V_{p,q}^{imp}(t) &= \langle\psi_p(x,y) \mid V_1(t) \mid \psi_q(x,y)\rangle \\ &= \sum_{nm}\sum_{n'm'} C_{nm,p}^* C_{n'm',q}\langle\phi_n(\alpha x)\phi_m(\beta y) \mid V_1(t) \\ &\mid \phi_{n'}(\alpha x)\phi_{m'}(\beta y)\rangle = V_0(t)\sum_{j=1}^{16} V_{p,q}^j(t) \end{aligned} \quad (5)$$