Journal of Physics and Chemistry of Solids 82 (2015) 76–81

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

Tuning diagonal components of static linear and first nonlinear polarizabilities of doped quantum dots by Gaussian white noise

Jayanta Ganguly [a], Manas Ghosh [b,*]

[a] Department of Chemistry, Brahmankhanda Basapara High School, Basapara, Birbhum 731215, West Bengal, India
[b] Department of Chemistry, Physical Chemistry Section, Visva Bharati University, Santiniketan, Birbhum 731 235, West Bengal, India

ARTICLE INFO

Article history:
Received 21 November 2014
Received in revised form
30 January 2015
Accepted 10 March 2015
Available online 11 March 2015

Keywords:
Electronic materials
Nanostructures
Quantum wells
Defects
Optical properties

ABSTRACT

We investigate the modulation of diagonal components of static linear (α_{xx}, α_{yy}) and first nonlinear (β_{xxx}, β_{yyy}) polarizabilities of quantum dots by Gaussian white noise. Quantum dot is doped with impurity represented by a Gaussian potential and repulsive in nature. The study reveals the importance of mode of application of noise (additive/multiplicative) on the polarizability components. The doped system is further exposed to a static external electric field of given intensity. As important observation we have found that the strength of additive noise becomes unable to influence the polarizability components. However, the multiplicative noise influences them conspicuously and gives rise to additional interesting features. Multiplicative noise even enhances the magnitude of the polarizability components immensely. The present investigation deems importance in view of the fact that noise seriously affects the optical properties of doped quantum dot devices.

1. Introduction

Development of new high-performance devices with promising optical properties has come out to be an important task of modern nanotechnology. The low-dimensional quantum systems are kind of modern devices which are highly renowned for displaying enhanced nonlinear optical effects than the bulk materials and possess widespread application in various optoelectronic devices. In consequence, we envisage an abundance of useful investigations on optical properties of these systems providing lots of information about the energy spectrum, the Fermi surface of electrons, and the value of electronic effective mass. Among the low-dimensional quantum systems, quantum dots (QD) are now recognized as prolific semiconductor optoelectronic devices. Furthermore, the presence of impurities strongly alters the optical properties of QD devices by virtue of extensive interplay between QD confinement sources and impurity potentials. Such alterations have successfully pampered new arenas of research in this field [1–11] with special emphasis on their linear and nonlinear optical properties [12–34].

External electric field has often been found to illuminate important aspects related with confined impurities. The electric field changes the energy spectrum of the carrier and controls the performance of the optoelectronic devices. Moreover, the electric field often hampers the symmetry of the system and facilitates emergence of nonlinear optical properties. Thus, the applied electric field assumes special attention in view of assiduous understanding of the optical properties of doped QDs [35–49].

Recently we have made extensive investigations of noise [50–52] as it influences the performances of QD devices. In these works we have analyzed the impact of *Gaussian white noise* on the *diagonal components* of *frequency-dependent* linear [50], first nonlinear [51], and the third nonlinear [52] polarizabilities of doped QD. In the present paper we examine the role of Gaussian white noise on the diagonal components of *static* linear (α_{xx}, α_{yy}) and first nonlinear (β_{xxx}, β_{yyy}) polarizabilities of doped QD which are still left unexplored. In the present study noise has been applied to the system *additively* and *multiplicatively* [50–52]. An external electric field of given intensity has been applied to the doped system which acts as a disturbance and generates linear and nonlinear responses. We have strived to elucidate the role of dopant location and the noise characteristics as they tailor the static diagonal polarizability components. The role of dopant site has been critically explored because of its sensitivity in shaping the optical properties of doped QDs. In their previous works Karabulut and Baskoutas [24] and Baskoutas et al. [35] highlighted the importance of off-center impurities and introduced a novel numerical method (*PMM*, *potential morphing method*). It needs to be mentioned that in one of our recent works [53] we have studied the frequency-dependent linear and nonlinear polarizabilities of doped QD whence the dopant was propagating under damped

* Corresponding author. Tel.: +91 3463 261526, +91 3463 262751x467; fax: +91 3463 262672.
E-mail address: pcmg77@rediffmail.com (M. Ghosh).

http://dx.doi.org/10.1016/j.jpcs.2015.03.011
0022-3697/

condition. However, in the present work damping as well as dopant propagation is not at all considered. Thus the environment is completely different. Moreover, frequency-dependent polarizabilities [53] bear widely different characteristics from that of static polarizabilities (in the present study). However, the basic methodologies in both the works are similar with some different equations arising out of different perturbing environments. The present analysis reveals the finer details in the profiles of aforesaid polarizability components as a result of intricate interplay between noise and the effective confinement potential. The effective confinement potential intimately depends on the site of dopant incorporation and thus the latter tunes the overall pattern of the polarizability components. Apart from this, the significance of mode of application of noise (additive/multiplicative) to the doped system has also been congruously addressed in the present paper.

2. Method

Our model Hamiltonian represents a 2-d quantum dot with single carrier electron laterally confined (parabolic) in the $x-y$ plane. The confinement potential reads $V(x, y) = \frac{1}{2}m^*\omega_0^2(x^2 + y^2)$, where ω_0 is the harmonic confinement frequency. The parabolic confinement potential has found extensive usage in various studies on QDs [1,4,5,8,9,14,22,37], particularly in the study of optical properties of doped QDs by Çakir et al. [20]. A perpendicular magnetic field ($B \sim$ mT in the present work) is also present as an additional confinement. Using the effective mass approximation we can write the Hamiltonian of the system as

$$H_0' = \frac{1}{2m^*}\left[-i\hbar\nabla + \frac{e}{c}A\right]^2 + \frac{1}{2}m^*\omega_0^2(x^2 + y^2). \tag{1}$$

In the above equation m^* stands for the effective electronic mass within the lattice of the material. The value of m^* has been chosen to be $0.067m_0$ resembling *GaAs* quantum dots. We have set $\hbar = e = m_0 = a_0 = 1$ and perform our calculations in atomic unit. In Landau gauge $[A = (By, 0, 0)]$ (A being the vector potential), the Hamiltonian transforms to

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

$\omega_c = eB/m^*c$ being the cyclotron frequency. $\Omega^2 = \omega_0^2 + \omega_c^2$ can be viewed as the effective frequency in the y-direction.

We now introduce impurity (dopant) to QD and the dopant is represented by a Gaussian potential [54–56]. To be specific, in the present case we write the impurity potential as $V_{imp} = V_0\, e^{-\xi\left[(x-x_0)^2+(y-y_0)^2\right]}$. Choice of positive values for ξ and V_0 gives rise to repulsive impurity. Among various parameters of impurity potential (x_0, y_0) denotes the dopant coordinate, V_0 is a measure of strength of impurity potential, and ξ^{-1} determines the spatial stretch of impurity potential. Recently Khordad and his coworkers introduced a new type of confinement potential for spherical QD's called *Modified Gaussian Potential, MGP* [57,58]. The Hamiltonian of the doped system reads

$$H_0 = H_0' + V_{imp}. \tag{3}$$

We have employed a variational recipe to solve the time-independent Schrödinger equation and the trial function $\psi(x, y)$ has been constructed as a superposition of the product of harmonic oscillator eigenfunctions [50–52] $\phi_n(px)$ and $\phi_m(qy)$ respectively, as

$$\psi(x, y) = \sum_{n,m} C_{n,m}\phi_n(px)\phi_m(qy), \tag{4}$$

where $C_{n,m}$ are the variational parameters and $p = \sqrt{m^*\omega_0/\hbar}$ and $q = \sqrt{m^*\Omega/\hbar}$. The general expressions for the matrix elements of H_0' and V_{imp} in the chosen basis have been derived [50–52]. In the linear variational calculation, requisite number of basis functions has been exploited after performing the convergence test. And H_0 is diagonalized in the direct product basis of harmonic oscillator eigenfunctions.

With the application of noise the time-dependent Hamiltonian becomes

$$H(t) = H_0 + V_1(t). \tag{5}$$

The noise consists of random term $(\sigma(t))$ which follows a Gaussian distribution (produced by Box–Muller algorithm) having strength μ. It is characterized by the equations: [50–52]

$$\langle\sigma(t)\rangle = 0, \tag{6}$$

the zero average condition, and

$$\langle\sigma(t)\sigma(t')\rangle = 2\mu\delta(t - t'), \tag{7}$$

the two-time correlation condition where the correlation time is negligible. The Gaussian white noise has been administered additively $[V_1(t) = \sigma(t)]$ as well as multiplicatively $[V_1(t) = \sigma(t)(x + y)]$ [50–52]. Experimentally, external noise can be generated by using a function generator (Hewlett-Packard 33120A) and its characteristics, Gaussian distribution and zero mean can be maintained [59]. The external noise could be introduced multiplicatively using a circuit that enables to drive the nonlinear element by using the voltage from an external source [60]. Hence the findings of current work can be made experimentally realizable and relevant.

The external static electric field V_2 of strength ϵ is now applied externally where

$$V_2 = \epsilon_x.\, x + \epsilon_y.\, y, \tag{8}$$

ϵ_x and ϵ_y are the field intensities along x and y directions, respectively. Now the time-dependent Hamiltonian reads

$$H(t) = H_0 + V_1(t) + V_2. \tag{9}$$

The matrix elements due to $V_1(t)$ and V_2 can be readily derived [50–52].

The evolving wave function can now be expressed by a superposition of the eigenstates of H_0, i.e.

$$\psi(x, y, t) = \sum_q a_q(t)\psi_q. \tag{10}$$

The associated time-dependent Schrödinger equation (TDSE) has now been solved numerically to obtain $\psi(x, y, t)$. For the numerical solution we have invoked sixth-order Runge–Kutta–Fehlberg method with a time step size $\Delta t = 0.01$ a.u. on verifying the numerical stability of the integrator. The time-dependent superposition coefficients $[a_q(t)]$ have been used to calculate the time-average energy of the dot $\langle E\rangle$ [50–52]. We have determined the energy eigenvalues for various combinations of ϵ_x and ϵ_y and used them to compute the diagonal components of linear and nonlinear polarizabilities by the following relations obtained by numerical differentiation:

$$\alpha_{xx}\epsilon_x^2 = \frac{5}{2}\langle E(0)\rangle - \frac{4}{3}\left[\langle E(\epsilon_x)\rangle + \langle E(-\epsilon_x)\rangle\right] + \frac{1}{12}\left[\langle E(2\epsilon_x)\rangle + \langle E(-2\epsilon_x)\rangle\right], \tag{11}$$