Physica B 468-469 (2015) 25–33

Contents lists available at ScienceDirect

Physica B

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

Fabricating off-diagonal components of frequency-dependent linear and nonlinear polarizabilities of doped quantum dots by Gaussian white noise

Surajit Saha [a], Jayanta Ganguly [b], Manas Ghosh [c,*]

[a] Department of Chemistry, Bishnupur Ramananda College, Bishnupur, Bankura 722122, West Bengal, India
[b] Department of Chemistry, Brahmankhanda Basapara High School, Basapara, Birbhum 731215, West Bengal, India
[c] Department of Chemistry, Physical Chemistry Section, Visva Bharati University, Santiniketan, Birbhum 731 235, West Bengal, India

ARTICLE INFO

Article history:
Received 4 December 2014
Accepted 7 April 2015
Available online 11 April 2015

Keywords:
Quantum dot
Impurity
Gaussian white noise
Frequency-dependent polarizability
Off-diagonal components
Dopant location

ABSTRACT

We make a rigorous exploration of the profiles of off-diagonal components of frequency-dependent linear (α_{xy}, α_{yx}), first nonlinear (β_{xyy}, β_{yxx}), and second nonlinear (γ_{xxyy}, γ_{yyxx}) polarizabilities of quantum dots driven by Gaussian white noise. The quantum dot is doped with repulsive Gaussian impurity. Noise has been applied additively and multiplicatively to the system. An external oscillatory electric field has also been applied to the system. Gradual variations of external frequency, dopant location, and noise strength give rise to interesting features of polarizability components. The observations reveal intricate interplay between noise strength and dopant location which designs the polarizability profiles. Moreover, the mode of application of noise also modulates the polarizability components. Interestingly, in case of additive noise the noise strength has no role on polarizabilities whereas multiplicative noise invites greater delicacy in them. The said interplay provides a rather involved framework to attain stable, enhanced, and often maximized output of linear and nonlinear polarizabilities.

1. Introduction

Quantum dots (QDs) are the substances where the process of miniaturization of semiconductor devices terminates. QDs display rich nonlinear optical effects which are much more delicate than the bulk materials. Thus, they have been ubiquitously applied as an indispensable ingredient in a variety of optical devices. Extensive study of optical properties of these devices endows us with lots of important information about their energy spectrum, the Fermi surface of electrons, and the value of electronic effective mass. These features have helped QDs earn wide recognition as high-performance semiconductor optoelectronic materials. However, QDs are frequently contaminated with dopants during their manufacture which dramatically alter their properties. As a result of contamination we envisage introduction of additional potential to the QD system which invariably interacts with intrinsic QD confinement potential. The interaction appears to be crucial for the dramatic change in various properties of QD. A large number of investigations on doped QD [1–15] therefore run in harmony with the increasing need of exploring their properties. Within the domain of optoelectronic applications, impurity driven modulation of linear and nonlinear optical properties has been found to be immensely important in photodetectors and in several high-speed electro-optical devices [16]. A plethora of important works on both linear and nonlinear optical properties of these structures was therefore a natural consequence [16–36].

External electric field has often been invoked to elucidate important aspects related with confined impurities. The electric field changes the energy spectrum of the carrier and modulates the performance of the optoelectronic devices. Moreover, the electric field often reduces the symmetry of the system and leads to emergence of nonlinear optical properties. Thus, the applied electric field assumes special attention in view of understanding the optical properties of doped QDs [37–53].

In some of our recent works we have made detailed discussions on importance of noise in influencing the performances of QD devices [54–56]. In these works we have explored the role of *Gaussian white noise* on the *diagonal components* of *frequency-dependent* linear [54], first nonlinear [55], and the second nonlinear [56] polarizabilities of doped QD. In the present manuscript we explore the role of *Gaussian white noise* on the *off-diagonal* components of *frequency-dependent linear* (α_{xy}, α_{yx}), *first nonlinear* (*second order*) (β_{xyy}, β_{yxx}), *and the second nonlinear* (*third order*)

* Corresponding author. Fax: +91 3463 262672.
E-mail address: pcmg77@rediffmail.com (M. Ghosh).

http://dx.doi.org/10.1016/j.physb.2015.04.009
0921-4526/

(γ_{xxyy}, γ_{yyxx}) polarizabilities of doped QD. The off-diagonal components require exploration as they interact differently with the applied field from their diagonal analogs and thus expected to display significantly distinct features. Of late Şahin made some important contribution to the third order optical property of a spherical QD and analyzed the role of impurity [22]. The notable works of Karabulut and Baskoutas [30] and Yilmaz and Şahin [34] also deserve mention in related contexts which include the effects of electric field and impurity. In the present study noise has been applied to the system *additively* and *multiplicatively* [54–56]. The polarizability components can be computed by applying an external electric field of given intensity to the doped system. We have put special emphasis on the role of dopant location and the noise characteristics as they modulate the off-diagonal polarizability components in some potentially interesting manner. The role of dopant site has been critically explored because of its well-known influence in modulating the optical properties of doped heterostructures. In their notable works Karabulut and Baskoutas [30], and Baskoutas et al. [37] analyzed the importance of off-center impurities exploiting an accurate numerical method (*PMM*, *potential morphing method*). Very recently Khordad and Bahramiyan have made important work on how dopant position affects the optical properties of various QDs [35]. The present analysis reveals the nuances in the profiles of aforesaid polarizability components as a result of intricate interplay between noise characteristics and the effective confinement potential of the doped QD system. The effective confinement potential has a strong dependence on the site of dopant incorporation and thus the latter makes a significant contribution in designing the overall profiles of the polarizability components. The impact of mode of application of noise (additive/multiplicative) on the polarizability components has also been critically addressed in the present manuscript.

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 [1,3,4,7–9,20,24,28,38,39], particularly in the study of optical properties of doped QDs by Çakir et al. [23,24]. 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 [57–59]. To be specific, in the present case we write the impurity potential as $V_{imp} = V_0 e^{-\xi\left[(x-x0)^2+(y-y_0)^2\right]}$. 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* [60,61]. 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 [54–56] $\phi_n(px)$ 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 [54–56]. In the linear variational calculation, a requisite number of basis functions have 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 [54–56]

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

the zero average condition, and

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

the two-time correlation condition with an insignificant correlation time. The Gaussian white noise has been administered additively [$V_1(t) = \sigma(t)$] as well as multiplicatively [$V_1(t) = \sigma(t)(x + y)$] [54–56].

The external electric field $V_2(t)$ of strength ϵ is now applied externally where

$$V_2(t) = \epsilon_x \cdot x \cdot \sin(\nu t) + \epsilon_y \cdot y \cdot \sin(\nu t) \tag{8}$$

ϵ_x and ϵ_y are the field intensities along x and y directions and ν being the oscillation frequency. Now the time-dependent Hamiltonian reads

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

The matrix elements due to $V_1(t)$ and $V_2(t)$ can be readily derived [54–56].

The evolving wave function can now be described 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 time-dependent Schrödinger equation (TDSE) carrying the evolving wave function has now been solved numerically by 6-th order Runge–Kutta–Fehlberg method with a time step size $\Delta t = 0.01$ a.u. after 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 $\langle E\rangle$ [54–56]. We have determined the energy eigenvalues for various combinations of ϵ_x and ϵ_y and used them to compute some of the