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# اثر ناهمسانگردی بر تغییرات ضریب شکست غیر خطی یک نقطه کوانتمی سه بعدی محدود شده در مرکز یک نانو سیم استوانه ای

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**چکیده- در این مقاله به بررسی اثر ناهمسانگردی هندسی بر تغیرات خطی و غیر خطی ضریب شکست یک نقطه کوانتمی که در مرکز یک نانو سیم استوانه‌ای قرار دارد با استفاده از روشهای تفاضلات محدود و ماتریس-چگالی پرداخته‌ایم. تغییرات ضریب شکست به صورت تابعی از انرژی فوتون تابشی و برای مقادیر متفاوت نسبت وجه نقطه سهموی و شعاع نقطه محاسبه شده‌اند. نتایج نشان می‌دهد که ناهمسانگردی هندسی نقش مهمی در تعین اندازه تغییرات غیر خطی ضریب جذب بازی می‌کند که ما را قادر به تنظیم حالت اشباع سیستم می‌کند. بعلاوه طیف اپتیکی سیستم به سمت انرژی های کمتر و بیشتر شیفت پیدا کرده که وابسته به شعاع نقطه کوانتمی و نسبت وجه آن می‌باشد.**

کلمات کلیدی: تغییرات ضریب شکست غیر خطی، نقطه کوانتمی ناهمسانگرد، نانو سیم.

# Anisotropy Effect on the Nonlinear Optical Refractive Index Changes of a Three-Dimensional Quantum Dot Confined at the Center of a Cylindrical Nano-wire

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Abstract-The effect of geometrical anisotropy is numerically investigated on the linear and nonlinear optical refractive index changes of a GaAs quantum dot which is located at the center of a $Ga_{1-x}Al_xAs$ cylindrical nano-wire. The finite difference approximation has been used for obtaining energy eigenvalues and corresponding wave functions. Also, the compact density matrix formalism is applied to investigate linear, third order nonlinear and total optical refractive index (RI) changes. The optical properties are calculated as a function of the incident photon energy for different ellipsoid aspect ratio and dot radius. The results clearly reveal that the dot anisotropy plays an important role in determining the magnitude of nonlinear RI changes which enable us to adjust saturation condition. We also found that the dot anisotropy shifts optical spectrum towards both lower and higher energies which depend on the shape of dot (spherical, prolate or oblate quantum dot) and dot radius.

Keywords: Nonlinear refractive index changes; Anisotropic quantum dot; Nano-wire.



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## 1 Introduction

In recent years, the nonlinear optical properties of semiconductor quantum dots (QDs) have been studied experimentally and theoretically [1]. The main reason is that for intersubband transitions the elements of dipole moment matrix are extremely large. Hence, the nonlinear terms of optical susceptibility are not negligible which enable us to apply QDs in the area of integrated optics and optical communications. In investigation of optical properties of QDs, most of the performed studies are related to linear and third order nonlinear refractive index (RI) changes [2, 3].
Recently, some researchers have studied electronic and optical properties of QDs with isotropic harmonic oscillator potential. It is shown that this type of potential is a more suitable suggested one due to this fact that the parabolic confinement is more appropriate when QD is fabricated [4]. On the other hand, a systematic study for anisotropic QDs is important as the Stranski–Krastanov QDs often display elliptic shape in the plane perpendicular to the growth axis which in turn significantly alters the physical properties [5]. Therefore, research on the anisotropic parabolic potential has attracted great attention, and the effects of the anisotropic parabolic potential on the energy eigenvalues and optical properties have been widely investigated [6,7].
Moreover, in the past decade, study of the electronic and optical properties of QDs has generally concerned self-assembled QDs. Developments in precise engineering make it possible to insert zero-dimensional QDs into one-dimensional nano-wires [8]. The one-dimensional geometry of the nano-wire has an important benefit which allows researchers to incorporate QDs in this active region and fabricate an interesting alternative to the self-assembled QDs. In this paper we present a numerical study of the linear and nonlinear optical RI changes in a three-dimensional anisotropic QD which is located at the center of a cylindrical nano-wire.

## 2 Theory

We consider a system consist of an electron in an anisotropic GaAs QD. The QD is located at the center of a $Ga_{1-x}Al_xAs$ cylindrical nano-wire with radius $R_2 = 20\,nm$ and height $l = 400\,nm$, the origin is taken at the bottom of the nano-wire and the z-direction is assumed to be along the nano-wire axis. In the effective mass approximation and in the cylindrical coordinates the Hamiltonian of a single particle can be expressed as

$$H = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}\right) + V^{AP} \quad (1)$$

Where $m^*$ is the band edge effective mass and the anisotropic parabolic confinement potential, $V^{AP}$, is given by [6]

$$V^{AP} = \frac{1}{2} m^* (\omega_\rho{}^2 \rho^2 + \omega_z^2 z^2) \quad (2)$$

Where $\omega_i (i = \rho, z)$ are the characteristic frequencies of an anisotropic three-dimensional parabolic potential. The Schrödinger equation is numerically solved by the finite difference (FD) approximation [9]. In order to carry out simulation, one needs to discretize Schrödinger equation using FD schemes. First it should be noted that in order to avoid achieving a huge coefficient matrix, the non-uniform space discretization is considered along z-coordinate with aspect ratio $\frac{\Delta z_{j+1}}{\Delta z_j} = \frac{z_{j+1} - z_j}{z_j - z_{j-1}} = 1.1$.
In order to calculate the optical properties of the system, we use the compact-density matrix approach and iterative procedure [2]. We consider the system subject to an electromagnetic field, $E(t) = \tilde{E} e^{i\omega t} + c.c$ , which is polarized along the z-direction. This electromagnetic field may cause an intersubband transition between an initial state, $i$, and a final state, $f$. Using the usual iterative procedure [2] the linear and third order nonlinear optical RI changes are given by

$$\frac{\Delta n^1(\omega)}{n_r} = \frac{1}{2n_r{}^2\varepsilon_0} \frac{\sigma_\nu |M_{fi}|^2 (E_{fi} - \hbar\omega)}{(E_{fi} - \hbar\omega)^2 + (\hbar\Gamma_{fi})^2}$$
(3)



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$$\frac{\Delta n^3(\omega)}{n_r} = -\frac{\mu c I}{4 n_r^3 \varepsilon_0} \frac{\sigma_\nu |M_{fi}|^2}{[(E_{fi}-\hbar\omega)^2 + (\hbar\Gamma_{fi})^2]^2} \times \left\{ 4(E_{fi}-\hbar\omega)|M_{fi}|^2 - \frac{(M_{ff}-M_{ii})^2}{E_{fi}^2 + (\hbar\Gamma_{fi})^2} \times [(E_{fi}-\hbar\omega)(E_{fi}(E_{fi1}-\hbar\omega) - (\hbar\Gamma_{fi})^2) - (\hbar\Gamma_{fi})^2(2E_{fi}-\hbar\omega)] \right\} \tag{4}$$

In Eqs. (3) and (4) $\varepsilon_0$ is the free-space electrical permittivity, $\sigma_\nu$ is the carrier density, c is the velocity of light in free space, μ is the magnetic permeability, $I = 2\varepsilon_0 n_r c|E|^2$ is the intensity of electromagnetic field, $M_{fi} = |<f|ez|i>|$ are the dipole moment matrix elements and $E_{fi} = E_f - E_i$ is the energy difference between *f*th and *i*th states. $\hbar\Gamma_{fi}$ are damping terms associated with the lifetime of the electrons [3].

## 3 Numerical results and discussion

In this section we study the linear and third order nonlinear RI changes of a GaAs anisotropic QD which is located at the center of a $Ga_{1-x}Al_xAs$ cylindrical nano-wire using the formulation developed in Section 2. All calculations were performed using the following parameters [10]: $m^* = 0.067 m_0$, $m_0$ is the mass of free electron, $\sigma_\nu = 5\times10^{24}\, m^{-3}$, $\varepsilon_r = 13.18$, $n_r = 3.63$ and $T_{fi} = 0.14\, ps$. The ellipsoid aspect ratio is indicated by $\eta = L_z / L_\rho = \sqrt{\omega_\rho / \omega_z}$ where $L_i = \sqrt{\hbar / m^* \omega_i}$. Hence, the ratio $\eta$ characterizes the degree of an isotropy of the QD. Also, the QD size is defined as the confinement characteristic length $R_1 = \sqrt[3]{L_\rho^2 L_z}$ which is called dot radius. It is important to point out that we just consider a two-level system and the intersubband transition occurs between ground and first excited states.

Fig. 1 shows the linear, third order nonlinear and total optical RI changes of the system as a function of the incident photon energy for spherical ($\eta = 1$), oblate ($\eta = 7$) and prolate ($\eta = 1.5$) QDs with radius $R_1 = 6\, nm$. It is clear that each RI curve has two extreme values. The region between these extreme values is called anomalous dispersion region and is defined as absorption band since the photon is strongly absorbed. The RI curves show red shift (blue shift) by a prolate (oblate) deviation from the spherical QD. The physical origin of this behavior is that by increasing ellipsoid aspect ratio energy difference between ground and first excited states reduces. Also, the magnitudes of linear and third order nonlinear RI changes increases as the ellipsoid aspect ratio increases. This behavior is a direct consequence of effect of ellipsoid aspect ratio on the dipole moment matrix elements. By increasing $\eta$ the dipole moment matrix of ground and first excited states increases which causes an increment in the total RI changes. On the other hand, by increasing $M_{fi}$ the nonlinear term of RI changes is also enhanced which is equivalent to this fact that the saturation in the system will occur at lower incident photon intensities.

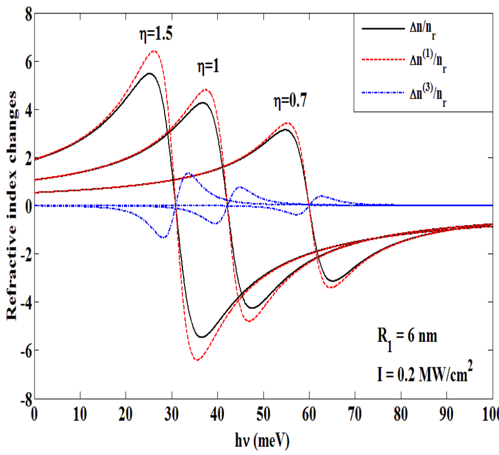


Fig. 1: The linear, third order nonlinear and total optical RI changes as a function of the incident photon energy for three different values of ellipsoid aspect ratio.

In order to see the effect of the size of QD on the optical properties, in Figs. 2 and 3 the linear, third order nonlinear and total RI



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changes have been plotted as a function of the incident photon energy for two different dot radii. In Fig. 2 RI changes are shown for oblate ellipsoidal QD with $\eta = 0.8$ whereas in Fig. 3 the same optical properties are plotted for a prolate ellipsoidal QD with $\eta = 1.5$. It is clear that for both oblate and prolate QDs by increasing the dot size the RI curves shifts toward lower energies. It is due to the energy difference between initial and final states decreases as the dot radius increases. Additionally, the magnitudes of linear and nonlinear terms increase by increasing the dot size, therefore, total changes in RI increase for all cases.

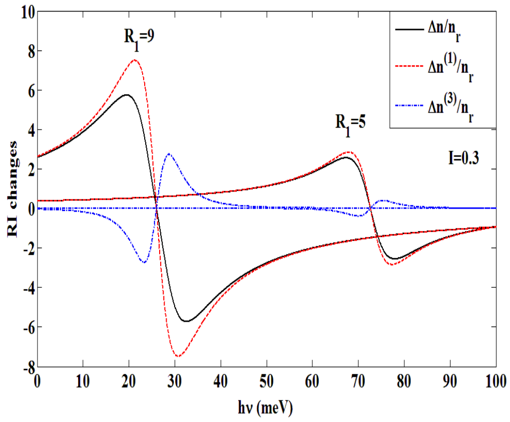


Fig. 2: The linear, third order nonlinear and total optical RI changes as a function of the incident photon energy for oblate QD with $\eta = 0.8$ and two different values of dot radius.

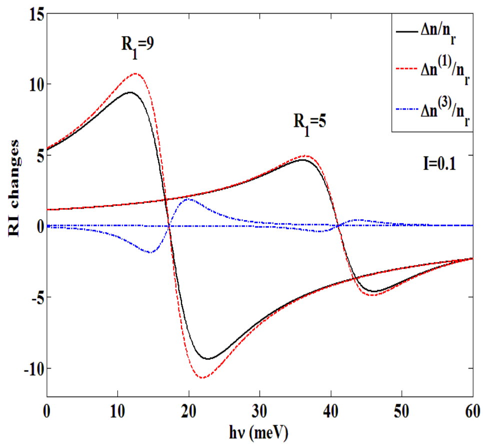


Fig. 3: The linear, third order nonlinear and total optical RI changes as a function of the incident photon energy for prolate QD with $\eta = 1.5$ and two different values of dot radius.

## 4 Conclusions

In conclusion, we have investigated the linear, third order nonlinear and total RI changes of a GaAs QD which is located at the center of a $Ga_{1-x}Al_xAs$ cylindrical nano-wire. The energy eigenvalues and wave functions are calculated by FD approximation and optical RI changes are calculated using compact density matrix formalism. Our results show that by increasing the dot radius or ellipsoid aspect ratio the optical spectrum shifts toward lower energies. Additionally, the magnitudes of linear and third order nonlinear RI changes have noticeably affected by prolate or oblate deviation from spherical QD and an augment in the dot radius.

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