# Effects of Plasma Interaction on a Random Array of Quantum Dots

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We calculated optical absorption coefficients for linear and monolayer arrays of ionized quantum dots (QD) of spherical or cylindrical shape with random dimensions and occupation numbers, obtained by Monte Carlo simulation. When submitted to an oscillating electric field each ionized QD behaves as a dipole and the interaction of them changes the form of the light absorption. The effect of the many electron system is considered by Density Functional Theory. The results obtained show a shift of the absorption peak to the right for increasing densities of QD's, whatever kind of shape or array of QD. Also absorption only, occurs when the electric field has a normal component to the array.

Keywords: Optical absorption coefficients; Arrays of ionized quantum dots; Effective mass approximation

## I. INTRODUCTION

The great progress in solid-state physics in the last two decades made it possible to reduce the dimensions of electronic systems, creating structures such as quantum wells, dots and wires and giving rise to important applications such as lasers, infrared detectors, etc [1]. In this article we deal with a random array of quantum dots (QD), distributed along a line or in a monolayer, Fig. 1, or in a multilayer in a semiconductor material, and submitted to an oscillating electric field. The QD's then act as electric dipoles and the interaction between then modify the free QD spectrum.
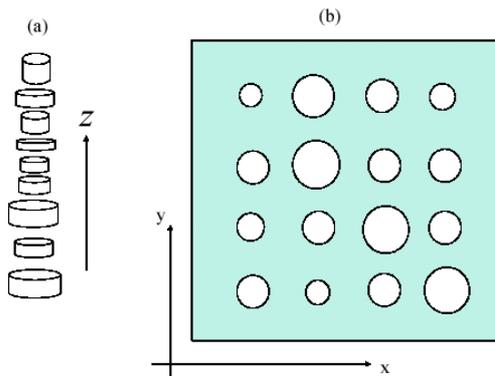


FIG. 1: (a) One-dimensional and (b) two-dimensional random arrays of cylindrical quantum dots.

The shapes of QD's studied here are cylindrical and spherical and the electronic wave functions are calculated using the method of Gangopadhyay and Nag[2], that may be used to calculate the envelope wave function of a QD of whatever shape.

The absorption coefficient is calculated via the method developed by Metzner et al [3,4], where the effect of the many electron system is considered by the Density Functional Theory[5].

The random aspect of this study is treated by Monte Carlo simulation [6].

## II. THEORY

The wave function of a single QD can be obtained in the effective mass approximation as a solution of the Hamiltonian eigenvalue equation due to Ben-Daniel and Duke [7]:

$$\left[ -\frac{\hbar^2}{2} \nabla \cdot \left( \frac{1}{m*(\mathbf{r})} \nabla \right) + V(\mathbf{r}) \right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \qquad (1)$$

where the effective mass $m*(\mathbf{r})$ and the potential $V(\mathbf{r})$ present discontinuities in the limits of the QD. The method of Gangopadhyay and Nag is the expansion of the envelope function $\Psi(\mathbf{r})$ in the base of functions formed by the eigenfunctions of a larger cubic QD of infinite potential barriers, Fig. 2.
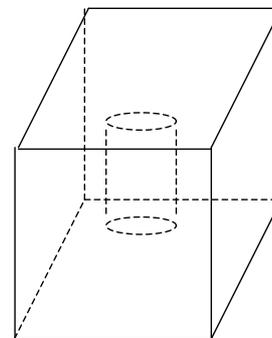


FIG. 2: A cylindrical QD in the center of a larger cubic QD.

For a system of QD's the interaction between them is taken into account by the Density Functional Theory, in which the potential $V(\mathbf{r})$ is replaced by the sum of it and a self-consistent potential $V^{(sc)}(\mathbf{r})$, function of the electronic density $n(\mathbf{r})$, written as:

$$V^{(sc)}(\mathbf{r}) = V_X(\mathbf{r}) + V_H(\mathbf{r}) \qquad (2)$$

where

$$V_X(\mathbf{r}) = -2e^2 \left( \frac{3n(\mathbf{r})}{8\pi} \right)^{1/3} \qquad (3)$$

is the exchange potential and

$$V_H(\mathbf{r}) = e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 r' \qquad (4)$$

is the Hartree potential, $e$ being the elementary charge. As in the case of a single QD the method of Gangopadhyay is used again while the self-consistency is completed.

We consider as a matter of simplification that each QD has only two states, the fundamental $\left|\Psi_0^{(I)}\right\rangle$ and the excited $\left|\Psi_1^{(I)}\right\rangle$, where $I$ is the index of the QD. The dipole moment of the $I^{th}$ QD excited with light polarized in the z direction is given by:

$$\mu_I = -ez^{(I)} = -e\left\langle \Psi_1^{(I)} \left| z \right| \Psi_0^{(I)} \right\rangle. \qquad (5)$$

The plasma interaction is then the direct and the exchange correlation interaction between the QD's. As one of them (J) performs the transition from the excited to the fundamental state it releases energy that is transferred to another one (I), which becomes excited.

Defining

$$\Delta n^{(J)}(\mathbf{r}) = \Psi_0^{(J)*}(\mathbf{r})\Psi_1^{(J)}(\mathbf{r}) \qquad (6)$$

as fluctuation on the electronic density due to the de-excitation of the $J^{th}$ QD, the induced fluctuation of the direct Coulomb potential is

$$\Delta D^{(J)}(\mathbf{r}) = \frac{1}{K} \int d^3 r_J \frac{1}{|\mathbf{r} - \mathbf{r}_J|} \Delta n^{(J)}(\mathbf{r}_J) \qquad (7)$$

where $K$ is dielectric constant of semiconductor in which are immersed the QD's.

The coupling strength between the $J^{th}$ and $I^{th}$ QD's, which corresponds to dipole-dipole interaction, is given by the matrix element

$$D^{(IJ)} = \left\langle \Psi_1^{(I)} \left| \Delta D^{(J)} \right| \Psi_0^{(I)} \right\rangle. \qquad (8)$$

In a analogous way is defined the strength of the exchange interaction

$$X^{(IJ)} = \left\langle \Psi_1^{(I)} \left| \Delta X^{(J)} \right| \Psi_0^{(I)} \right\rangle, \qquad (9)$$

where, in the local density functional approximation,

$$\Delta X^{(J)}(\mathbf{r}) = \left[ \frac{dV_X}{dn} \right]_{n=n(\mathbf{r})} \Delta n^{(J)}(\mathbf{r}). \qquad (10)$$

For each QD is defined a response function in terms of the angular frequency of incident light $\omega$, the transition energy

to the excited state $\Delta E_{10}^{(I)}$ and a parameter $\Gamma$ that accounts for homogeneous broadening of the resonance line:

$$R^{(I)}(\omega) = \frac{1}{\Delta E_{10}^{(I)} - \hbar\omega - i\Gamma} \qquad (11)$$

The amplitudes of oscillation $A^{(I)}(\omega)$ for the QD are solutions of a linear system of equations that presents couplings between oscillators:

$$\sum_J \left[ \delta_{IJ} - R^{(I)}(\omega)\left( D^{(IJ)} - X^{(IJ)} \right) \right] A^{(J)}(\omega) = E_0 \mu_I R^{(I)}(\omega) \qquad (12)$$

where $E_0$ is the amplitude of the incident electric field.

The absorption coefficient [8,9] is calculated from these amplitudes. Since

$$\alpha(\omega) = Re\left(\sigma(\omega)\right) = \frac{\omega}{4\pi} Im\left(\varepsilon(\omega)\right), \qquad (13)$$

$$\varepsilon(\omega) - 1 = 4\pi \frac{P(\omega)}{E(\omega)} \qquad (14)$$

and

$$P(\omega) \propto \sum_I A^{(I)}(\omega), \qquad (15)$$

where $\sigma$ is the optical conductivity, $\varepsilon$ is the complex dielectric function and $P$ is the electric polarization, we finally have

$$\alpha(\omega) \propto \omega \sum_I Im[A^{(I)}(\omega)] \qquad (16)$$

## III. SPECIFICATIONS OF THE SYSTEM

We consider arrays of cylindrical InAs QD's immersed in GaAs, with effective masses given by 0.040 and 0.0665 respectively and confining potential of 450 meV [10] due to the difference between the conduction band edges of the two materials. The parameter $\Gamma$ was chosen to be equal to 1.0 meV while the dimensions of the QD's to have gaussian randomic dispersion so that the broadening in the absorption line is 20 meV.

The radius and the height of a QD of finite potential barrier are chosen in a way there is at least one excited state that could be populated by the action of the oscillating electric field, furthermore the dipole moment (5) must be not zero in order that the absorption occurs. For a linear array grown in the z direction it was considered a disk-type QD with an electric field applied in the x direction. The medium radius and height were 10.8 nm and 2.1 nm respectively, being 3.2 nm the mean distance between them. For a mono-layer of QD's placed in the

xy it was used a can-type QD with an electric field normal to the layer. This simulation was made with medium radius, height and distance between them equal to 3.1 nm, 30.0 nm and 7.2 nm respectively.

The randomness in these arrays is taken into account of the dimensions of QD's, the distance between them, the occupation number of bound electrons, here taken as zero or one. The algorithm used was Monte Carlo Simulation [6] that consists in generation of pseudo random numbers to simulate different configurations of the system.

## IV. RESULTS AND CONCLUSIONS

In Fig. 3 is represented the Hartree (8) and exchange (9) interaction energy between QD's in a linear array in function of their distance showing the major effect of the Hartree potential. This energy is positive and its effect on the absorption coefficient is to shift the peak to the right and narrowing it as the electronic density increases, see Figs. 4 and 5. It seems to be an universal property that does not depend on the type of array, the shape of the QD or the materials that form the system. The results are the same when the GaAs spherical QD's are formed in AlAs [11] as it should be since the shape and dimensions of a QD are responsible for the energy levels while the shift on the peak occurs due to the interaction between the QD's.
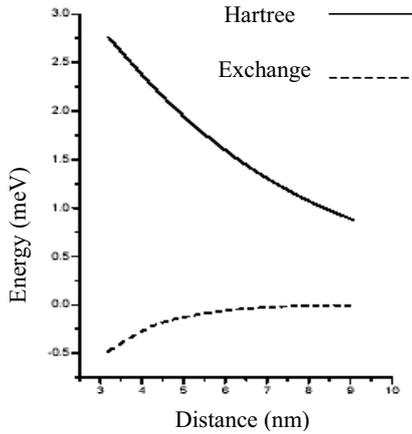
FIG. 3: Hartree and exchange energy between QD's.

It should be noted that the electric field must have a normal component to the array because the QD's dimensions in that direction could be greater than the ones in the plane or line of QD's so that the fundamental and at least some excited states are present and the resonance could take place.

Although this effect occurs in linear and planar arrays of QD's the response to the applied field is more intense in planar arrays since it depends on the total number of QD's in the material.

It is interesting to note that the classical interaction between dipoles ($\mathbf{p}_1$ and $\mathbf{p}_2$) is given by
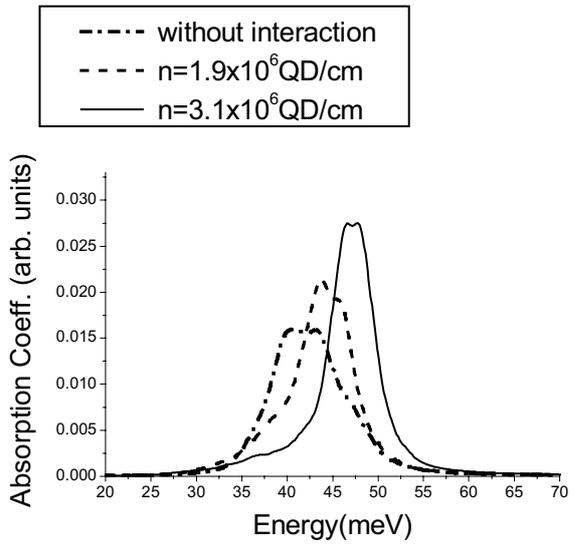
FIG. 4: Absorption coefficient for a linear array of QD'in function of density of QD's.
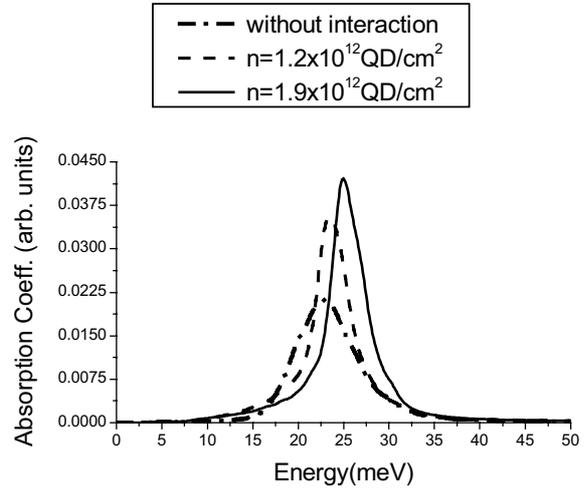
FIG. 5: Absorption coefficient for a mono-layer of QD'in function of the density of QD's.

$$U_{12} = \frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{r^3} - \frac{3\mathbf{r} \cdot \mathbf{p}_1 \mathbf{r} \cdot \mathbf{p}_2}{r^5} \qquad (17)$$

where $\mathbf{r}$ is the vector joining the two dipoles. For the case in which

$$\mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p} \qquad (18)$$

and $\theta$ is the angle between $\mathbf{r}$ and $\mathbf{p}$

$$U_{12} = \frac{p^2}{r^3} (1 - 3\cos\theta) \qquad (19)$$

so $U_{12}$ may be positive or negative in an apparent contradiction the results of this work. This fact can be explained remembering that the dipole moments are parallel to the electric field and it must have a normal component to the array, then $U_{12}$ is always positive justifying this calculation.

Although this effect is subtle we hope it will be possible to be measured in the not too distant future.

[1] J. Faist, F. Capasso, L. Sivco, C. Sirtori, A Hutchinson, and A. Chou, Science **264**, 553 (1994).

[2] S. Gangopadhyay and B. R. Nag, Nanotechnology **8**, 14 (1997).

[3] C. Metzner and G. H. Döhler, Phys. Rev. B **60**, 11005 (1999).

[4] R. N. Riemann, C. Metzner and G. H. Döhler, Phys. Rev. B **65**, 115304 (2002).

[5] E. K. U. Gross, *Many Particle Theory*, Adam Hilger, (1992).

[6] J. M. Thijssen, *Computational Physics,* Cambridge University Press, 1999.

[7] D. J. Ben-Daniel and C. B. Duke, Phys. Rev. **152**, 683 (1966).

[8] J. N. Hodgson, *Optical Absorption and Dispersion in Solids*, Chapman and Hall LTD, London (1970).

[9] E. de P. Abreu, Doctoral Thesis, UFSCar (2004).

[10] M. Califano and P. Harrison, Phys. Rev. B **61**, 10959 (2000).

[11] E. de P. Abreu and P. D. Emmel, *Proceedings of CIMTEC 2002 , International Conference of Modern Materials and Technologies,* Florence, Italy, July 2002.