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Polarizability with an effect of an Electric field for a donor in spherical GaAs QDs

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Abstract:- In this present work, first I simplified and calculated the binding energy of a donor in spherical quantum dots (QDs) by using a variational approach within the effective mass approximation and computed for GaAs QD as a function of the dot size for different impurity positions. Next I found out the expectation value of the Hamiltonion and also the binding energies were computed for different values of the electric fields. I found that the value of the polarizability obtained is several orders higher than the hydrogen atom value. My results are in good agreement with previous theoretical findings.

Keywords:- Spherical quantum dot, Donor binding energy, Impurity state, Parabolic confinement Quantum dots , quantum wells gallium arsenide, III-V semiconductors, impurity states, effective mass, donor Binding , Semiconductor compounds, Polarizability of atoms, Polarizability of molecules.
PACS, 73.20.Dx , 73.20.Hb ,73.21.La , 73.21.-b , 73.61.Ey , 73.20.Hb , 71.18.+y, 71.38.+I , 71.20.Nr, 32.10.Dk, 33.15.Kr

I. INTRODUCTION

Recently, the evolution of the growth techniques such as molecular beam epitaxy and metal-organic chemical vapor deposition combined with the use of the modulation-doped technique made it possible the fabrication of low-dimensional heterostructures such as single and multiple quantum wells, quantum wires, and quantum dots. In these systems, the restriction on the motion of the charge carriers allows us to control the physical properties of the structures. The studies on these systems offer a wide range of potential applications in the development of semiconductor optoelectronic devices [19-23].

GaInNAs/GaAs quantum well (QW) lasers have been attracting significant scientific interest mainly due to their applications in 1.3- or 1.55-μm optical fiber communication [24-30]. These lasers are predominantly based on GaInAsP alloys on the InP substrates, which have a higher temperature sensitivity compared to shorter wavelength lasers that are grown on GaAs substrates. The high-temperature sensitivity is primarily due to Auger recombination and the weak electron confinement resulting from the small conduction band offset in the GaInAsP/InP material system.

GaInNAs alloys grown on GaAs substrates have been proposed as a possible alternative to the GaInAsP/InP system for achieving lasers with high-temperature performance [31]. The deeper conduction band well and the larger electron effective mass will provide better confinement for electrons and better match of the valence and conduction band densities of state, which leads to a higher characteristic temperature and higher operating temperature, higher efficiency, and higher output power [24-30].

The purpose of this work is to investigate the effect of an applied electric field on the binding energies of shallow donor impurities GaAs QDs. The dimensions and the geometry of the system that we have used in our work can be considered quite realistic due to the continuous development of the nm-structuring processes (see,for example, Schweizer et al. [14]).

The results for the binding energy and polarizability in the effective-mass approximation,using a variational scheme given and also given the values of the polarizability with an effect of an electric field for a shallow hydrogenic donor in spherical GaAs QDs.
My results are in good agreement with previous theoretical findings.

The paper is organized as follows: in the 'Theoretical overview' section, the essential theoretical background is described.

The next important section is the 'Introduction about Polarizability' section, and finally, my calculations are given and 'Conclusions' section.

This work gives very important information about the binding energy and polarizability that can be taken into account in experimental work related to absorption processes,and carrier dynamics, associated with impurities in these heterostructures.

The Hamiltonian of a single hydrogenic impurity in a spherical QD with parabolic confinement in the effective mass approximation [2] can be written as

$$H= [P^2/2m^*] +1/2 [m^*\omega^2r^2] – e^2 / \varepsilon|(r-r_i)|$$

Where e and m^* are, respectively, the electronic charge and effective mass, P is a momentum, ω is a characteristic frequency, ε is the dielectric constant of the dot material, and r_i gives the location of the impurity with respect to the center of the dot.

In order to calculate the ground state of the impurity binding energy, the variational technique is used[3], and for this the trial wave function is taken as

$$\psi (r) = N(\lambda) \exp(-\beta r^2 /2) \exp(-\lambda|(r-r_i)|) ,$$

Where $\beta=m^*\omega /h /2\pi$. Here h being the Planck's constant. λ is the variational parameter and $N(\lambda)$ is the normalization constant. The ground state energy of the hydrogenic impurity is worked out from the above equations by using the below relation.

$$E(\lambda,\beta,r_i) = <\psi^* /H/ \psi> / <\psi^* /\psi>$$

Here ψ^* means the conjugate of the eigen function ψ.

II. THEORY

We first derived the binding energy for two cases:

$r_i = 0$., ie., the location of the impurity is zero.
$r_i = a$ .r., ie., impurity at the inner surface of the dot.

In **case I**, at $r_i = 0$, the location of the impurity is zero.

Therefore the Hamiltonian of a single hydrogenic impurity in a spherical QD with parabolic confinement can be written as

$$H= [P^2/2m] +1/2 [m^*\omega^2r^2] – e^2 / \varepsilon|(r-r_i)|$$

The trial wave function is taken as

$$\psi (r) = N(\lambda) \exp(-\beta r^2 /2) \exp(-\lambda|(r-r_i)|) ,$$

Where $\beta=m^*\omega /h /2\pi$. Here h being the Planck's constant. λ is the variational parameter and $N(\lambda)$ is the normalization constant.

Normalization condition: $<\psi^* /\psi> = 1$

By equating everything, we get

$$\int\psi(r) [1/2 m^*\omega^2r^2] \psi(r) d\tau = 2\pi N^2 e^2 e^{\lambda/\beta} / m^* [\lambda(\text{sqrt}(\pi)) / \beta^{3/2 -} 1/2\beta]$$

This is the final solution for case (i). Then the binding energy will be,

$$<E> = 2\pi N^2h^2 e^{\lambda/\beta} /m^* \{-5 (\text{sqrt}(\pi)) /2\beta^{1/2}\} - \ldots\ldots$$

By using this the binding energy was computed for GaAs QD as a function of the dot size.

When $\beta^{-1/2}$ (nm) = 2, then <E> in Ryd* = 13.1. When $\beta^{-1/2}$ (nm) = 10, then <E> in Ryd* = 3.0.

*1 Ryd = 5.3 meV for GaAs

In this the present works are compared with the values of the references . Finally a graph is drawn between the impurity binding energy versus the dot size. As the size -→ ∞ , the energy should 1 Ryd.

In **Case II, a**t r_i = a, the location of the impurity is at the inner surface of the dot.

Therefore the Hamiltonian of a single hydrogenic impurity in a spherical QD with parabolic confinement can be written as

$H= [P^2/2m^*] +1/2 [m^*\omega^2r^2] – e^2 / \varepsilon|(r-a)|$

The trial wave function is taken as

$\psi (r) = N(\lambda) \exp(-\beta r^2 /2) \exp(-\lambda|(r-a)|)$,

Where $\beta=m^*\omega /h /2\pi$. Here h being the Planck's constant. λ is the variational parameter and $N(\lambda)$ is the normalization constant.

Normalization condition: $<\psi^* /\psi> = 1$

By equating everything, we get

$$\int\psi(r) [1/2 m^*\omega^2r^2] \psi(r) d\tau = 2\pi N^2 e^2 e^{\lambda/\beta} / m^* [\lambda(sqrt(\pi)) / \beta^{3/2} - (2 \lambda/ \beta) +(1/2\beta) - .....]$$

This is the final solution for case (i). Then the binding energy will be,

$<E> = 2\pi N^2h^2 e^{\lambda/\beta} /m^* \{25 (sqrt(\pi)) /8\beta ^{½}\}$ - ……

By using this the binding energy was computed for GaAs QD as a function of the dot size.

When $\beta^{-1/2}$ (nm) = 2, then <E> in Ryd* = 12.0. When $\beta^{-1/2}$ (nm) = 10, then <E> in Ryd* = 3.8.

*1 Ryd = 5.3 meV for Ga As

In this the present works are compared with the values of the references .

Finally a graph is drawn between the impurity binding energy versus the dot size. For the case r_i = a.

Comparisons of the <E> values, it reveals that the binding energy is larger in the case where the impurity is at the centre of the dot.

III. POLARIZABILITY WITH AN EFFECT OF AN ELECTRIC FIELD

Introduction

Neutral nonpolar species have spherically symmetric arrangements of electrons in their electron clouds. When in the presence of an electric field, their electron clouds can be distorted (**Figure**). The ease of this distortion is defined as the polarizability of the atom or molecule. The created distortion of the electron cloud causes the originally nonpolar molecule or atom to acquire a dipole moment. This induced dipole moment is related to the polarizability of the molecule or atom and the strength of the electric field by the following equation:

$\mu_{ind} = \alpha' E$

Where E denotes the strength of the electric field and α' is the polarizability constant with units of C m^2 V^{-1}.

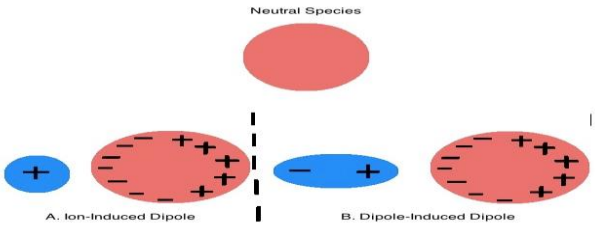


Figure: A neutral nonpolar species's electron cloud is distorted by A.) an Ion and B.) a polar molecule to induce a dipole moment.

With the electrons held tightly in place in these smaller atoms, these atoms are typically not easily polarized by external electric fields.

In contrast, large atoms with many electrons, such as negative ions with excess electrons, are easily polarized. These atoms typically have very diffuse electron clouds and large atomic radii that limit the interaction of their external electrons and the nucleus.

Factors that Influence Polarizability

The relationship between polarizability and the factors of electron density, atomic radii, and molecular orientation is as follows:

- The greater the amount of electrons, the less control the nuclear charge has on charge distribution, and thus the increased polarizability of the atom.
- The greater the distance of electrons from nuclear charge, the less control the nuclear charge has on the charge distribution, and thus the increased polarizability of the atom.
- Molecular orientation with respect to an electric field can affect polarizibility (labeled Orientation-dependent), except for molecules that are: tetrahedral, octahedral or icosahedral (labeled Orientation-independent).

This factor is more important for unsaturated molecules that contain areas of electron dense regions, such as 2,4-hexadiene. Greatest polarizability in these molecules is achieved when the electric field is applied parallel to the molecule rather than perpendicular to the molecule.

Polarizability with an effect of an Electric field for a shallow hydrogenic donor in spherical GaAs QDs with parabolic confinement

The effect of an applied electric field on the binding energies of shallow donor impurities in rectangular cross section GaAs quantum-well wires (QWW) was presented by Montes et al. [3],

considering an infinite confinement potential and using a variational scheme. Quantum-mechanical calculations of the carrier densities,elect ron and hole quasi-Fermi-levels,and various radiative decay times in rectangular transversal-section GaAs QWWs have been performed under steady-state cw-laser excitation conditions [13].

They considered the effects of the cw-laser intensity,the temperature,the physical dimensions of the structure,an d a homogeneous distribution of electron-traps in the system.

The theoretical results for the laser-intensity-dependent quasi- Fermi-levels were found to be in qualitative agreement with available experimental data [14]. However,the numerical data show that further experimental and theoretical work is necessary.

In addition,there have been several reports on the polarizabilities of shallow-donor impurities in QWs and in surface QWWs [15-18].

The presence of an external electric field in rectangular cross section QWWs modifies the impurity band due to the fact that the field breaks the energy degeneracy for symmetrical impurity positions along the transversal section of the wires. This is reflected by additional peaks in the impurity DOIS and in the absorption and photoluminescence spectra.

I studied above theories and done the calculation for the polarizability with an effect of an electric field for a shallow hydrogenic donor in spherical GaAs QDs with parabolic confinement, following variational procedure within the effective mass approximations.

The computed result shows that the binding energy increases as the dot size decreases.

In the present work I investigate the effect of an applied electric field on the binding energies of shallow donor impurities GaAs QDs. The dimensions and the geometry of the system that we have used in our work can be considered quite realistic due to the continuous development of the nm-structuring processes (see,for example, Schweizer et al. [14]).

I present the results for the binding energy and polarizability in the effective-mass approximation,using a variational scheme for the infinite-confinement potential model and yield the values of the polarizability with an effect of an electric field for a shallow hydrogenic donor in spherical GaAs QDs.

The donor atom in our system in an external electric field is given by,

$$H= [P^2/2m] +1/2\ [m^*\omega^2r^2] - e^2 / \varepsilon|(r-r_i)| + \varepsilon ez$$

We use the trial wave function, $\psi(r) = N(\lambda) \exp(-\beta r^2/2) \exp(-\lambda|(r-a)|) (1+\alpha ez)$

where $z = r\cos\vartheta$. And α is treated as a variational parameter.

In the case of 'On- Centre ' impurity ($r_i = 0$), the normalization condition yields,

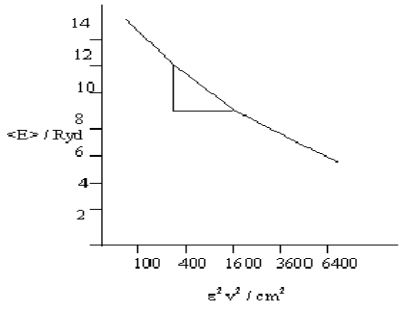
$N^2 = 1 / 4\pi \; e^{\lambda/\beta} \; [[sqrt(\pi)/\beta^{3/2}(\ldots) \; ^{-} \; \lambda/ \beta[1+(\varepsilon^2\alpha^2)/3] +(\lambda^{2}/ \beta^{5/2}) (\ldots) - \ldots..]$

If we put $\alpha = 0$, then we get the N^2 value for case 1. (i.e., $r_i = 0$)

I simplified this for second case also and I found out the expectation value of the Hamiltonion and also the binding energies were computed for different values of the electric fields.

The results are presented in the below Table.

Graph



Using these datas, a graph was drawn for binding energy Vs ε^2, (see in figure).

The curve is linear. However for small values of ε, it is linear and gives the value of α_p as $0.7 * 10^2 * (10^{-24}\ cm^3)$ for polarizability which is defined as

Table

$\beta^{-1/2}$ (nm)	**<E> in Ryd***				
	ε =0	**ε =10**	**ε =20**	**ε =40**	**ε =60**
2	13.18	13.48	13.47	13.46	13.44
4	12.10	12.42	12.39	12.35	12.27
6	7.93	8.16	8.12	8.10	8.02
8	4.99	5.42	5.39	5.37	5.26
10	3.18	3.57	3.49	3.46	3.38

*1 Ryd = 5.3 meV for Ga As

$\alpha_p = [\partial <E> / \partial \varepsilon^2] |_{\varepsilon=>0} = 0.7 * 10^2 * (10^{-24}\ cm^3)$

IV. CONCLUSION

We have presented a calculation for the polarizability with an effect of an Electric field for a shallow hydrogenic donor in spherical GaAs QDs with parabolic confinement, following variational procedure within the effective mass approximations. The computed result shows that the binding energy increases as the dot size decreases. In spherical quantum dots, with an isotropic parabolic potential, the impurity binding energy is found to decrease as the impurity moves away from the center, the effect being more pronounced for dots of smaller sizes.

REFERENCE BOOKS

[1] Bastard G 1981 Phys.Rev.B24 4714
[2] Chayanika Bose , 1998 J,Appl. Phys. 83 3089
[3] Sakaki H 1981 J.Vac.Sci. Technol. 19 148
[4] Vojak B.A., Laidig W.D, Holonyak N.Camras M D, Coleman J J and Dapkus
[5] Schiff. L. I. (1968) Quantum Mechanics, III rd Edition, Phys.265
[6] Lorke, J.P.Kotthaus, and K.Ploog, phys.Rev. Lett. 64 , 2559(1990)

[7] Petrucci, Ralph H., et al. General Chemistry: Principles and Modern Applications.Upper Saddle River, NJ: Prentice Hall, 2007, http://www.chem.purdue.edu/gchelp/liquids/disperse.html
[8] http://chemed.chem.purdue.edu/genchem/topicreview/bp/ch8/valenceframe.html
[9] Chang, Raymond. "Chapter 13: Intermolecular Forces/ Ion-Induced Dipole and Dipole-Induced Dipole Interactions/ Dispersion, or London, Interactions." Physical Chemistry for the Biosciences. Sansalito, CA: University Science, 2005. 495-98. Print.
[10] Housecroft, Catherine E., and Alan G. Sharpe. "Chapter 6: Structures and Energetics of Metallic and Ionic Solids." Inorganic Chemistry. Harlow [etc.: Prentice Hall, 2008. 173-74. Print.
[11] Miessler, Gary L., and Donald A. Tarr. "Chapter 6: Acid-Base and Donor-Acceptor Chemistry." Inorganic Chemistry. Upper Saddle River, NJ: Pearson Education, 2004. 183-86. Print.
[12] "Polarizability." Chemical Education at University of Wisconsin. Web. 14 Mar. 2011. <http://chemed.chem.wisc.edu/chempath...ility-859.html>.
[13] C.A. Duque,C.A.C. Mendonc¸a,L.E. Oliveira,Proceedings of the II Workshop on Optoelectronic Materials and Their Applications (Including Solar Cells),La Habana–
[14] Cuba,November 2–6,1998, pp. 130–132.
[15] H. Schweizer,G. Lehr,F. Prins,G. Mayer, E. Lach, R. Kr.uger,E. Fr.ohlich,M.H. Pilkuhn,G.W. Smith,Superlatt. Microstruct. 12 (1992) 419.
[16] M. El-Said,M. Tomak,Phys. Stat. Sol. B 171 (1992) K29.
[17] V. Narayani,B. Sukumar, Solid State Commun. 90 (1994) 579.
[18] H. Thien Cao,D.B. Tran Thoai, Solid State Commun. 97 (1996) 643.
[19] K.F. Ilaiwi,Superlatt. Microstruct. 20 (1996) 173.
[20] Reed MA. Quantum dots. Sci Am. 1993;268:118.
[21] Loss D, DiVicenzo DP. Quantum computation with quantum dots. Phys Rev A. 1998;57:120. doi: 10.1103/PhysRevA.57.120. [Cross Ref]
[22] Jiang X, Li SS, Tidrow MZ. Study of intersubband transition in quantum dots and quantum dot infrared photodetectors. Physica E. 1999;5:27. doi: 10.1016/S1386-9477(99)00026-0. [Cross Ref]
[23] Kristaedter N, Schmidt OG, Ledentsov NN, Bimberg D, Ustinov VM, Yu A, Zhukov AE, Maximov MV, Kopev PS, Alferov ZI. Gain and differential gain of single layer InAs/GaAs quantum dot injection lasers. Appl Phys Lett. 1996;69:1226. doi: 10.1063/1.117419. [Cross Ref]
[24] Imamura K, Sugiyama Y, Nakata Y, Muto S, Yokoyama N. New optical memory structure using self-assembled InAs quantum dots. Jpn J Appl Phys. 1995;34:L1445. doi: 10.1143/JJAP.34.L1445. [Cross Ref]
[25] Kondow M, Uomi K, Niwa A, Kitatani T, Watahiki S, Yazawa Y. GaInNAs: a novel material for long-wavelength-range laser diodes with excellent high-temperature performance. Jpn J Appl Phys. 1996;35:1273. doi: 10.1143/JJAP.35.1273. [Cross Ref]
[26] Kondow M, Kitatani T, Nakahara K, Tanaka T. A 1.3 μm GaInNAs laser diode with lifetime of over 1000 hours. Jpn J Appl Phys. 1999;38:L1355. doi: 10.1143/JJAP.38.L1355. [Cross Ref]
[27] Kitatani T, Nakahara K, Kondow M, Uomi K, Tanaka T. A 1.3 μm GaInNAs/GaAs single-quantum well laser diode with high characteristic temperature over 200 K. Jpn J Appl Phys. 2000;39:L86. doi: 10.1143/JJAP.39.L86. [Cross Ref]
[28] Tansu N, Yeh JH, Mawst LJ. Low-threshold 1317-nm InGaAsN quantum-well lasers with GaAsN barriers. Appl Phys Lett. 2003;83:2512. doi: 10.1063/1.1613998. [Cross Ref]
[29] Gonul B, Oduncuoglu M, Dindaroglu S, Yagdiran B. Influence of doping on gain characteristics of GaInNAs/GaAs quantum well lasers. Semicond Sci Technol. 2003;18:163. doi: 10.1088/0268-1242/18/2/318. [Cross Ref]
[30] Galluppi M, Geelhaar L, Reichert H. Nitrogen and indium dependence of the band offsets in InGaAsN quantum wells. App. Phys Lett. 2005;86:131925. doi: 10.1063/1.1898441. [Cross Ref]
[31] Tansu N, Quandt A, Kanskar M, Mulhearn W, Mawst LJ. High-performance and high-temperature continuous-wave-operation 1300 nm InGaAsN quantum well lasers by organometallic vapor phase epitaxy. Appl PhysLett. 2003;83:18.
[32] Kondow M, Kitatani T, Nakatsuka S, Larson MC, Nakahara K, Yazawa Y, Okai M. GaInNAs: a novel material for long-wavelength semiconductor lasers. IEEE J Sel Top Quantum Electron. 1997;3:719. doi: 10.1109/2944.640627. [Cross Ref]