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Shape effect of diamagnetic susceptibility of a hydrogenic donor in a nano structured semiconductor systems

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Abstract The diamagnetic susceptibility of a hydrogenic donor in GaAs/ $Al_xGa_{1-x}As$ semiconductor nanostructured systems like Quantum Well Wire and Quantum Dot has been computed for various cross-sectional geometries of these systems for various width of the confining potential in the effective mass approximation using variational method. The non parabolicity of the conduction band has also been included. This calculation may throw some light on the effect of geometries on the semiconductor–metal transition in these systems.

Keywords Hydrogenic donor · Quantum Well Wire · Quantum Dot · Diamagnetic susceptibility

1 Introduction

Impurity states in a semiconductor nanostructured system like Quantum Well (QW), Quantum Well Wire (QWW), and Quantum Dot (QD) has drawn a considerable interest during the past few decades [1–8] due to technological applications and also due to novel phenomena exhibited by them. One of the effects addressed by Bryant [5] was the effect of shape of these systems on the hydrogenic impurity states in QWW as the coulomb problem in these nanostructures are intriguing and the binding energy of hydrogenic impurities strongly depends on the dimension and geometry of the sample. Kasapoglu et al. [9] have also studied the geometrical effects on shallow donor impurities in QWW. Extending the impurity state problem to determine the diamagnetic susceptibility of a donor in these systems, Nithiananthi and Jayakumar [10,11] have reported the same in the literature. Further, the same authors [12] have recently

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demonstrated the semiconductor–metal transition in QW by finding an abrupt change in diamagnetic susceptibility at a critical concentration which agrees very well with the experimental result [13]. In the light of Bryant's work, [5] it is interesting to investigate how the diamagnetic susceptibility (χ_{dia}) is affected by the (cross-sectional) geometry of the QWW and QD within the effective mass approximation. We hope such investigation would throw more light on the effect of geometry on the semiconductor–metal transition in semiconducting nanostructured systems. We present the theory and then results and discussions in the subsequent sections.

2 Theory

The Hamiltonian of the donor impurity in GaAs/$Al_xGa_{1-x}As$ nanostructured systems in the effective mass approximation is given in atomic units by

$$\mathbf{H} = \frac{-\nabla^2}{2m^*} - \frac{1}{\varepsilon_0 r} + V_B(r) \tag{1}$$

where m* is the effective mass of the electron in GaAs well and ε_0 is the static dielectric constant of GaAs. The non parabolicity of the conduction band [10] is included through energy dependent effective mass as

$$m^* = m\left[1 + \frac{\gamma(E)}{m}\right] \tag{2}$$

where $\gamma(E) = 0.0436\,E + 0.236\,E^2 - 0.147\,E^3$ and E is in eV.

The infinite potential barrier height of the Quantum Well Wire and Quantum Dot is given by

$$V_B(r) = \begin{cases} 0 & |x| \le \frac{L_x}{2}, |y| \le \frac{L_y}{2} \\ \infty & \text{otherwise} \end{cases} \quad \text{for Quantum Well Wire} \tag{3a}$$

$$V_B(r) = \begin{cases} 0 & |x| \le \frac{L_x}{2}, |y| \le \frac{L_y}{2}, |z| \le \frac{L_z}{2} \\ \infty & \text{otherwise} \end{cases} \quad \text{for Quantum Dot} \tag{3b}$$

where L_x, L_y and L_z give the dimension of the system along x, y and z axes.

The ground state wavefunction of a donor is given as

$$\Psi_{QWW} = \begin{cases} N_{QWW} \cos\frac{\pi x}{L_x} \cos\frac{\pi y}{L_y} e^{-\alpha_{QWW} r} & |x| \le \frac{L_x}{2}, |y| \le \frac{L_y}{2} \\ 0 & \text{otherwise} \end{cases} \tag{4a}$$

$$\Psi_{QD} = \begin{cases} N_{QD} \cos\frac{\pi x}{L_x} \cos\frac{\pi y}{L_y} \cos\frac{\pi z}{L_z} e^{-\alpha_{QD} r} & |x| \le \frac{L_x}{2}, |y| \le \frac{L_y}{2}, |z| \le \frac{L_z}{2} \\ 0 & \text{otherwise} \end{cases} \tag{4b}$$

where $r = \sqrt{x^2 + y^2 + z^2}$; N_i (i = QWW, QD) is the normalization constant and α_i is the variational parameter which is different in each case.

The Schrödinger equation is solved variationally and $\langle H \rangle_{min}$ is determined to fix the wavefunction Ψ_i through the variational parameter α_i.

The diamagnetic susceptibility (χ_{dia}) of the hydrogenic donor [10] is given by

$$\chi_{dia} = -\frac{1}{6m^*\varepsilon_0 c^2}\left\langle r^2 \right\rangle \tag{5}$$

where c is the velocity of light (=137 and e = 1, $m_o = 1$ in atomic units) and $\left\langle \Psi_i \right| r^2 \left| \Psi_i \right\rangle$ is the mean square distance of the electron from the nucleus.

3 Results and discussions

The various cross sectional geometries of the QWW are defined as $G_j(x, y)$: $G_1(L, L)$, $G_2(L, L/2)$ and $G_3(L/2, L/4)$ and for QD as $G_j(x, y, z)$: $G_1(L, L, L)$, $G_2(L, L/2, L)$ and $G_3(L/2, L/4, L)$.

The variational parameters for the QWW and QD for various geometries and for both parabolic and non parabolic cases are presented in Tables 1 and 2, respectively. Since the calculation of χ_{dia} involves $\langle r^2 \rangle$, we present the same for both QWW and QD in Fig. 1a and b, respectively for various cross sectional geometries G_j. The variation of χ_{dia} against well width for both QWW and QD and for various geometries are given in Fig. 2a and b respectively.

Table 1 Variational parameters for a QWW in parabolic and non parabolic cases for various cross sectional geometries

L(Å)	Parabolic			Non parabolic		
	G_1	G_2	G_3	G_1	G_2	G_3
50	0.0084	0.0094	0.0122	0.0106	0.0149	0.0238
100	0.0065	0.0073	0.0094	0.0068	0.0086	0.0149
150	0.0055	0.0063	0.0081	0.0057	0.0068	0.0106
200	0.0052	0.0058	0.0073	0.0052	0.006	0.0086
300	0.0045	0.0051	0.0063	0.0047	0.0053	0.0068

Table 2 Variational parameters for a QD in parabolic and non parabolic cases for various cross sectional geometries

L(Å)	Parabolic			Non parabolic		
	G_1	G_2	G_3	G_1	G_2	G_3
50	0.0024	0.0028	0.0039	0.0042	0.0066	0.0117
100	0.0025	0.0029	0.004	0.003	0.0041	0.0085
150	0.0026	0.003	0.004	0.0028	0.0035	0.0062
200	0.0027	0.0031	0.004	0.0028	0.0034	0.0053
300	0.0029	0.003	0.0041	0.003	0.0034	0.0046

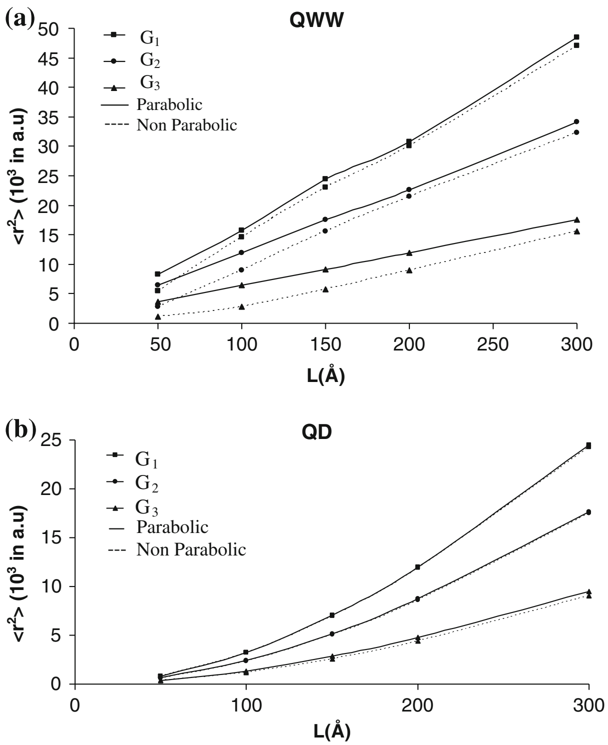

Fig. 1 (**a**) Variation of $\langle r^2\rangle$ with well width for a Quantum Well Wire for various geometries for both parabolic and non parabolic cases. (**b**) Variation of $\langle r^2\rangle$ with well width for a Quantum Dot for various geometries for both parabolic and non parabolic cases

From these figures, it is observed that χ_{dia} is higher for QD than for QWW. It is also observed that χ_{dia} increases as the cross sectional geometry decreases for both QWW and QD. This may be because of the squeezing of the wavefunction as the geometry decreases, which enhances χ_{dia}. This trend has been reflected in the plot $\langle r^2\rangle$ against L in Fig. 1a and b. It is to be noted that in the bulk limit, $\langle r^2\rangle \rightarrow 3a_B{}^{*2}$ ($1\ a_B{}^* \sim 100$Å) which in turn causes $\chi_{dia} \rightarrow -1.13$ a.u, agreeing with our earlier results [10]. Unfortunately, as no theoretical or experimental results are available, we could not compare our result.

It is understandable that the non parabolicity introduced through the energy dependent effective mass (m*) also increases the χ_{dia} for lower cross sectional geometries and for lower well width L in the case of a QWW. Though a similar feature has been observed in QD, the effect is lower.

To conclude, the cross sectional geometry of the QWW and QD and also the non parabolicity of the conduction band has a significant effect on χ_{dia}. As mentioned earlier, we hope that it will be possible to demonstrate the effect of cross sectional geometry on the semiconductor–metal transition through χ_{dia} in these nanostructured systems.

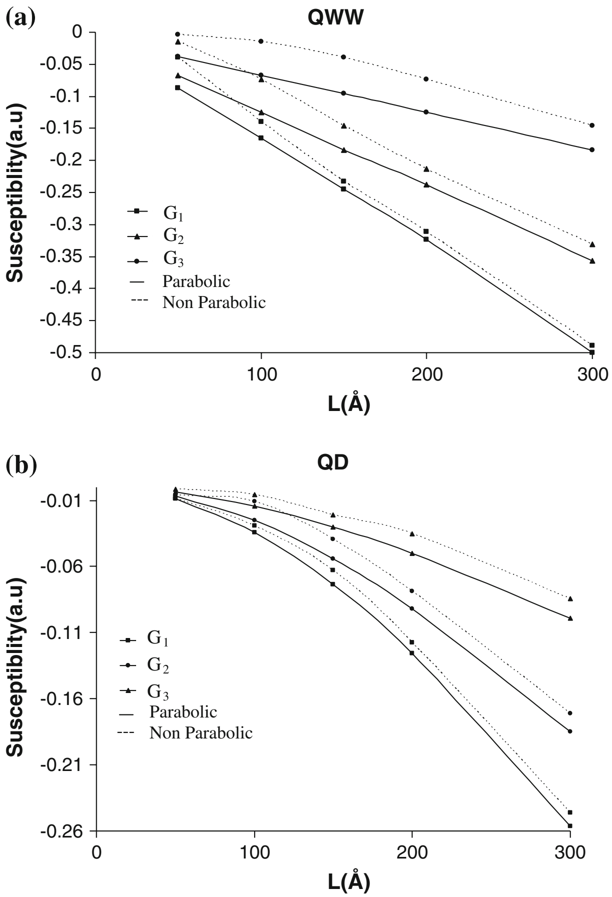

Fig. 2 (**a**) Variation of χ_{dia} with well width for a Quantum Well Wire for various geometries for both parabolic and non parabolic cases. (**b**) Variation of χ_{dia} with well width for a Quantum Dot for various geometries for both parabolic and non parabolic cases

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