Pressure dependence of the diamagnetic susceptibility of a donor in low-dimensional semiconductor systems

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The pressure dependence of the donor ionization energy (E_{ion}) and diamagnetic susceptibility (χ_{dia}) are calculated for quasi-two-dimensional (Q2D), quasi-one-dimensional (Q1D), and quasi-zero-dimensional (Q0D) semiconductor systems consisting of GaAs quantum wells with $Ga_{1-x}Al_xAs$ barriers forming a superlattice system. The results we arrived at are as follows: E_{ion} increases with pressure for a given well width (L), for a given magnetic field (B), and for a given system (Q2D, Q1D, or Q0D); E_{ion} increases with magnetic field for a given L, for a given P, and for a given system; χ_{dia} decreases with an increase in pressure and χ_{dia} decreases when the spatial dimension of the system is reduced for a given L and P.

I. INTRODUCTION

Low-dimensional semiconductor systems (LDSS) are drawing considerable attention at present. The literature is rich with works on quantum wells (quasi-two-dimensional, Q2D), quantum well wires (quasi-one-dimensional, Q1D) and quantum dots (quasi-zero-dimensional, Q0D).[1-4] Doped semiconductor systems under an external perturbation such as our electric field or a magnetic field are of most relevance to device fabrications and applications. Having been motivated by the computation[5] and the subsequent measurement[6] of χ_{dia} for doped Si, especially its relevance to the metal-insulator transition, the present work is devoted to the computation of donor ionization energies and diamagnetic susceptibilities of LDSS under the influence of external pressure. An analogous problem of donor polarizabilities in a quantum well,[7,8] in a quantum well wire[9] (QWW), and in quantum box[10] have recently drawn considerable attention.

II. THEORY

The Hamiltonian of the system (neglecting spin) consisting of a donor electron kept at the center of the well (in GaAs) formed by band offsets at the junctions of GaAs and $Ga_{1-x}Al_xAs$ in Q2D, Q1D, and Q0D systems under the influence of an external magnetic field is

$$H=-\frac{\hbar^2}{2m^*}\nabla^2-\frac{e^2}{4\pi k_0\epsilon r}+V(\mathbf{r})+\frac{e}{2m^*}(\mathbf{B}\cdot\mathbf{L})+\frac{e^2A^2}{2m^*}, \tag{1}$$

where K_0 is the permittivity of free space, L is the orbital angular momentum, and $\mathbf{A}=\frac{1}{2}\mathbf{B}\times\mathbf{r}$ is the vector potential. m^* is the band mass pertinent to the conduction-band minimum in GaAs and ϵ is the static dielectric constant. We have

$$V(x,y,z)=\begin{cases}0\,, & \text{for } |z|<\frac{L}{2}\,,\quad |x|\,\&\,|y|<\infty\\ \infty\,, & \text{otherwise (Q2D)}\end{cases}$$
$$=\begin{cases}0\,, & \text{for } |x|<\frac{L}{2}\,,\quad |y|<L/2\,\&\,|z|<\infty\\ \infty\,, & \text{otherwise (Q1D)}\end{cases}$$
$$=\begin{cases}0\,, & |x|\,,|y|\,,|z|<L/2\\ \infty\,, & \text{otherwise (Q0D)}\end{cases} \tag{2}$$

for different systems. The confining geometries are a square well in Q2D, a two-dimensional square well in Q1D (wire with a square cross section), and three-dimensional square well in Q0D (a quantum box of cubic geometry). The effect of external hydrostatic pressure (P) on the effective mass is considered through an approximate formula[11]

$$\frac{m}{m^*}\simeq 1+\frac{2\hbar^2}{ma_l^2E}\,,$$

where m^* is the band mass, and a_l is the lattice constant, and E is the average band gap, all of which vary with pressure. The variation of band gap with pressure is given by[12]

$$E(P)=(1.45+0.12P-3.77\times10^{-3}P^2)\text{ eV}\,,$$

where P is expressed in GPa. The variation of dielectric constant with pressure is taken from[13] $\epsilon(P)=12.56-0.088P$ where P is again expressed in GPa. The variation of the lattice constant with pressure is given by Balkemore.[12] We express the width of the well (L) as $L(P)=kL(0)$ where $k=[a_l(P)/a_l(0)]$ in which $a_l(P)$ is the lattice constant at a given pressure and $a_l(0)$ is the lattice constant at atmospheric pressure. The values of $\epsilon(P)$, $m^*(P)$, and k are given in Table I. In what follows we drop the P in parentheses and designate these quantities as ϵ, m^*, and k only.

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TABLE I. Pressure variation of certain characteristic parameters of GaAs.

P (GPa)	ϵ	m^*	$k=[a_l(P)/a_l(0)]$
0[a]	12.560	0.0680	1
1	12.472	0.0728	0.9961
2	12.384	0.0772	0.9922
3	12.296	0.0810	0.9881
4	12.208	0.0845	0.9840

[a]This refers to atmospheric pressure.

In the case of a quantum well, choosing the variational ansatz

$$\phi_1=N_1\exp[-(x^2+y^2)/8a^2]\exp(-z^2/8b^2)\cos(\pi z/L) \tag{3}$$

with a and b as the variational parameters and the normalization constant $N_1=(8\pi a^2 I_1)^{-1/2}$ and choosing the magnetic field along the Z axis, the ground-state energy is given by

$$\langle H\rangle=R_1+R_2+R_3+R_4 \tag{4}$$

where

$$R_1=\left\langle -\frac{\hbar^2}{2m^*}\nabla^2\right\rangle =\frac{\hbar^2}{2m^*}\left[\frac{1}{4a^2}+\frac{1}{16b^4}\frac{I_3}{I_1}+\frac{\pi^2}{L^2}\frac{I_2}{I_1}+\frac{\pi}{4Lb^2}\frac{I_4}{I_1}-\frac{\pi^2}{L^2}\right],$$

$$R_2=\left\langle -\frac{e^2}{4\pi K_0\epsilon r}\right\rangle=-\frac{e^2}{16\pi^2K_0\epsilon a^2}\frac{I_5}{I_1},$$

$$R_3=\left\langle \frac{e}{2m^*}\mathbf{B}\cdot\mathbf{L}\right\rangle=0,$$

$$R_4=\left\langle \frac{e^2A^2}{2m^*}\right\rangle=\frac{e^2B^2a^2}{2m^*}.$$

The ionization energy is obtained from

$$E_{\text{ion}}=E_1+E_L-\langle H\rangle_{\min}$$

where $E_1=\hbar^2\pi^2/2m^*L^2$ and the Landau level is given by $E_L=\hbar\omega_c/2$ with the cyclotron frequency $\omega_c=eB/m^*$.

Similar expressions have been obtained for the cases of a QWW and a quantum box. The trial wave functions chosen are

$$\phi_2=N_2\exp[-(x^2+y^2)/8b^2]\exp(-z^2/8a^2)\times\cos(\pi x/L)\cos(\pi y/L) \tag{5}$$

TABLE II. Variational parameters a and b (in Å) for different well widths (L), magnetic fields (B), and pressures (P). The values given are for atmospheric pressure. Quantities within parentheses refer to 4 GPa.

L (Å)	B (T)	Q2D a	Q2D b	Q1D a	Q1D b	Q0D a	Q0D b
100	0	42	161	27	76	43	43
		(34)	(114)	(23)	(60)	(38)	(38)
	1	42	161	27	76	43	43
		(34)	(114)	(23)	(60)	(38)	(38)
	2	42	161	27	76	43	43
		(34)	(114)	(23)	(60)	(38)	(38)
	5	40	152	26	73	43	43
		(34)	(114)	(23)	(60)	(38)	(38)
200	0	49	126	37	82	58	58
		(41)	(94)	(32)	(66)	(50)	(50)
	1	49	126	37	82	58	58
		(41)	(94)	(32)	(66)	(50)	(50)
	2	48	124	37	82	58	58
		(41)	(94)	(32)	(66)	(50)	(50)
	5	46	118	37	81	58	58
		(39)	(89)	(32)	(65)	(49)	(50)
500	0	63	105	56	91	76	76
		(52)	(78)	(47)	(70)	(59)	(59)
	1	63	105	56	91	76	76
		(52)	(78)	(47)	(70)	(59)	(59)
	2	61	102	55	89	74	75
		(51)	(76)	(47)	(69)	(58)	(59)
	5	54	92	51	80	67	73
		(47)	(71)	(44)	(64)	(55)	(57)

for a QWW and

$$\phi_3 = N_3 \exp[-(x^2+y^2)/8a^2]\exp(-z^2/8b^2)\cos(\pi x/L) \times \cos(\pi y/L)\cos(\pi z/L) \quad (6)$$

for a quantum box. N_2 and N_3 are the normalization constants. The magnetic field is applied along the [110] axis in a QWW and along the [001] axis in the quantum box. The lowest subband energies in these two cases are $\hbar^2\pi^2/m^*L^2$ (QWW) and $3\hbar^2\pi^2/2m^*L^2$ (quantum box). Since the infinite-well approximation is used, it follows that ϕ_1, ϕ_2, and ϕ_3 are zero outside the wells.

The diamagnetic susceptibility is given by

$$\chi_{\text{dia}} = -\frac{e^2a^2}{m^*}(\text{quantum well})$$
$$= -\frac{e^2}{4m^*}\left[2a^2 + \frac{I_3}{I_1}\right](\text{QWW}) \quad (7)$$
$$= -\frac{e^2}{2m^*}\frac{I_6}{I_7}(\text{quantum box}) .$$

The above expressions are obtained from the coefficients of B^2 in the corresponding energy expressions given above. These give directly $-\frac{1}{2}\chi_{\text{dia}}$ in each case. In the above expressions $I_1 \cdots I_7$ are certain integrals which are given in the Appendix. The values of a and b in Eq. (7) correspond to magnetic fields that are low. In the numerical work, the binding energy of an electron for a few low magnetic fields are obtained. The values of a and b do not change appreciably for these low fields (see Table II). This procedure amounts to plotting binding energy versus B^2 and taking the slope as $B \to 0$ in the estimation of χ_{dia}.

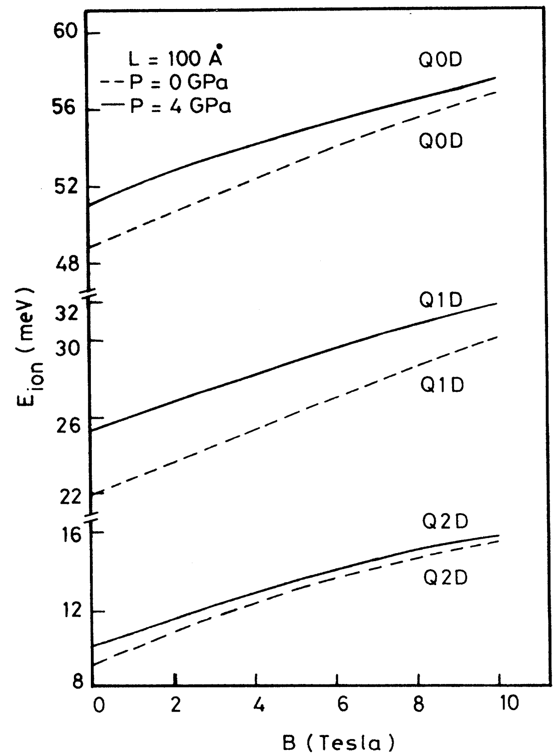

FIG. 2. Variation of the donor ionization energy with magnetic field in LDSS for $P = 0$ and 4 GPa when the well width is 100 Å.

III. RESULTS AND DISCUSSION

The results of our calculation are presented in Figs. 1–5. From Fig. 1 we conclude that (i) for a given B and

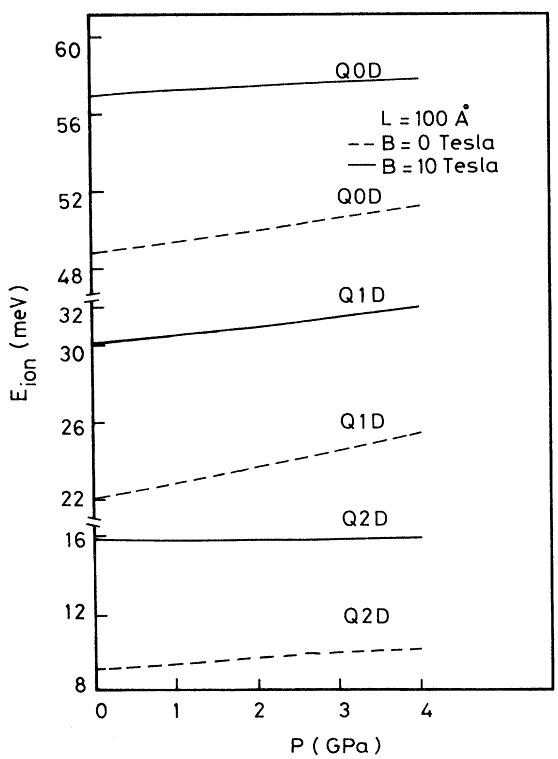

FIG. 1. Donor ionization energy vs pressure in LDSS for $B = 0$ and 10 T when the well width is 100 Å.

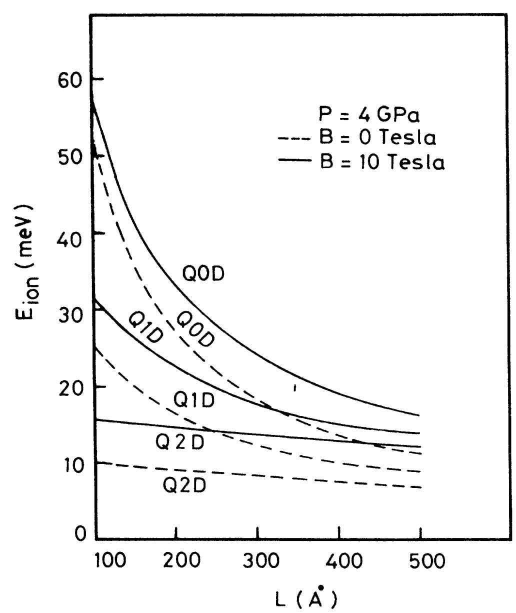

FIG. 3. Variation of the donor ionization energy with well width in LDSS for $B = 0$ and 10 T at $P = 4$ GPa.

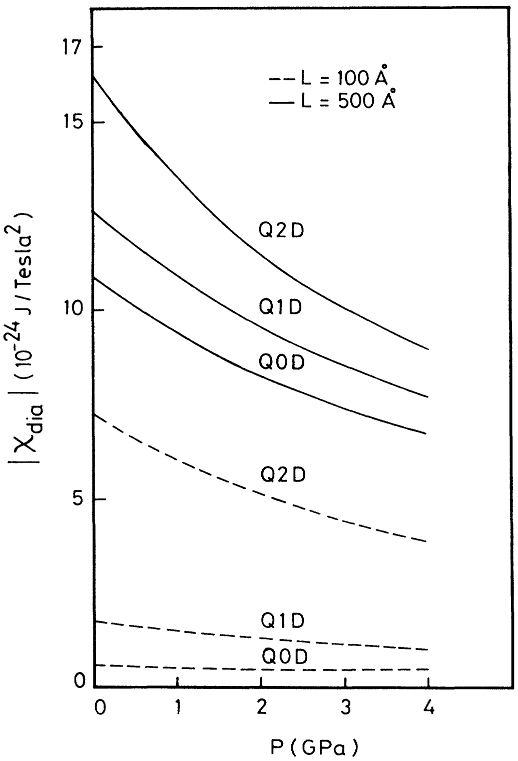

FIG. 4. The magnitude of the diamagnetic susceptibility vs pressure in LDSS for two different well widths.

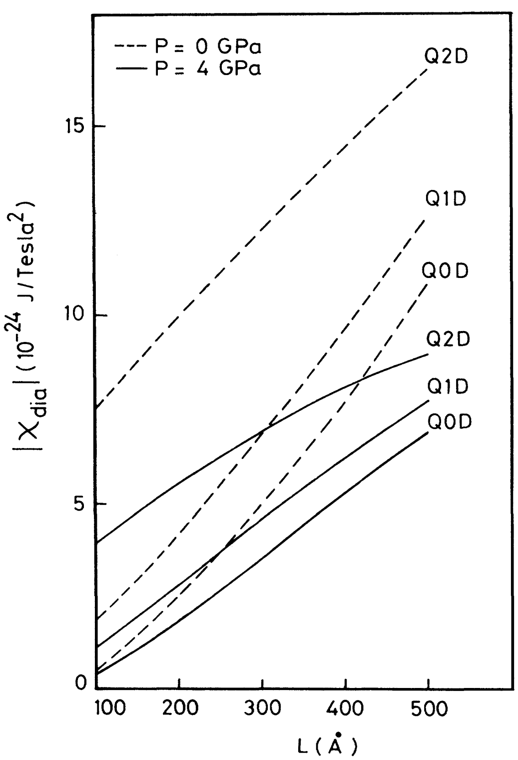

FIG. 5. Variation of the magnitude of the diamagnetic susceptibility with well width in LDSS for $P=0$ and 4 GPa.

L, E_{ion} increases with P in all three systems, and (ii) increasing the magnetic field increases the ionization energy for a given P, a result which is evident from Fig. 2 as well. Our results for a quantum well are in agreement with Ref. 14. Results for a QWW are in agreement with Ref. 9. The effect of the pressure is seen to be larger for lower magnetic fields.

Figure 3 shows the variation of E_{ion} with L for a given P. It is seen that E_{ion} decreases with L in all three cases. This result is well known for zero pressure in all three systems.[14–16] Increasing the magnetic field for a given P and L increases E_{ion} as noted in Fig. 2 also.

The variation of $|\chi_{dia}|$ with pressure is presented in Fig. 4. It is seen that $|\chi_{dia}|$ decreases with pressure. Increasing the well width increases the value of $|\chi_{dia}|$ also for a given P in all three systems, the increase being more prominent for low pressures. Figure 5 shows the variation of $|\chi_{dia}|$ with L. It is clearly seen that $|\chi_{dia}|$ increases with L as noted in Fig. 4 also. Increasing P for a given L decreases the value of $|\chi_{dia}|$ in all three systems. It is also seen that the variation of P on $|\chi_{dia}|$ is the largest in Q2D and this variation is more prominent for larger L values. It is believed that, as the expressions for χ_{dia} given above for the three cases reveal, this is due to the reduction in the lateral orbital dimension (a) when external pressure is applied. In the other two cases, χ_{dia} depends in a more complicated way on both a and b parameters.

In the present work, pressures above 4 GPa are not considered. It is well known that near this pressure GaAs becomes an indirect-band-gap material.[17] In such a situation the use of the simple effective-mass theory is questionable,[18] the complications arising due to the many valley nature of the conduction-band minimum.

At present there do not exist any experimental or other theoretical estimates of χ_{dia}. So we are unable to compare our results. It is hoped that the measurement of χ_{dia} will throw further light on the nature of the ground state, especially the ground-state wave function.

APPENDIX

The Integrals $I_1 \cdots I_7$ are given in the following:

$$I_1=\int_0^{L/2}\exp(-x^2/4b^2)\cos^2(\pi x/L)dx \ ,$$

$$I_2=\int_0^{L/2}\exp(-x^2/4b^2)dx \ ,$$

$$I_3=\int_0^{L/2}\exp(-x^2/4b^2)\cos^2(\pi x/L)x^2dx \ ,$$

$$I_4=\int_0^{L/2}\exp(-x^2/4b^2)\sin(2\pi x/L)xdx \ ,$$

$$I_5=\int_{x=-\infty}^{\infty}\int_{y=-\infty}^{\infty}\int_{z=0}^{L/2}\exp[-(x^2+y^2)/4a^2] \times\exp(-z^2/4b^2) \times\cos^2(\pi z/L)\frac{1}{r}dx\,dy\,dz \ .$$

I_6 and I_7 are I_3 and I_1, respectively, in each of which b is replaced by a.

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