Dielectric response to a donor ion in a $Ga_{1-x}Al_xAs$-GaAs-$Ga_{1-x}Al_xAs$ quantum well of infinite depth

P. Csavinszky and A. M. Elabsy
Department of Physics, University of Maine, Orono, Maine 04469
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We consider the dielectric response to a donor ion in a GaAs quantum well of infinite depth in two cases: (1) The ion is placed at the center of the well; (2) the ion is placed into off-center positions in the well. In each of these cases we calculate the binding energy of the donor atom as a function of the width of the well and compare our values with those arising from Bastard's theory, where the donor atom is considered as a hydrogenic impurity. We find that consideration of the dielectric response of the GaAs quantum well leads to important deviations with respect to Bastard's hydrogenic theory. Specifically, we find that, in case (1), our binding energies at different well widths are larger in magnitude than those calculated from Bastard's theory. We also find that the discrepancy between the two sets of binding energies is a function of the width of the well, becoming less pronounced as the width of the well is increased. We further find that, in case (2), as the donor atom is moved from the center of the well toward the wall of the well, our binding energies at different well widths rise toward those calculated from Bastard's theory and practically merge with them at a certain impurity position. We analyze our findings, and conclude that the dielectric response in a narrow GaAs quantum well is an important factor in the theory of impurity states in the well.

I. INTRODUCTION

A superlattice consists of alternating layers of two different semiconductors with well-defined layer thicknesses and sharp interfaces between the layers. One of the superlattices that has received considerable recent attention is made of alternating layers of $Ga_{1-x}Al_xAs$ and GaAs. This structure exhibits periodic discontinuities of the conduction bands (and valence bands) at the interfaces between the alternating layers. For $x \lesssim 0.4$, the conduction-band mismatch is such that an electron in a GaAs layer is confined to a potential well whose height depends on the x value of the two neighboring $Ga_{1-x}Al_xAs$ layers.[1] Such a GaAs layer, sandwiched between two $Ga_{1-x}Al_xAs$ layers, is referred to as a quantum well.

The first study of hydrogenic impurity states in a GaAs quantum well, considered to be of infinite depth, is due to Bastard.[2] (With the assumption of infinite well depth, the $Ga_{1-x}Al_xAs$-GaAs-$Ga_{1-x}Al_xAs$ superlattice can be considered as a set of independent quantum wells.) Bastard[2] has carried out variational calculations to determine the binding energy of a donor atom both as a function of the GaAs layer thickness and the position of the donor atom in the GaAs quantum well. In the calculations of Bastard,[2] the image charges on the interfaces arising from dielectric mismatch between the layers have been neglected, and, in the spirit of the hydrogenic approximation, the Coulomb interaction energy between the donor ion and the donor electron has been scaled by the static dielectric constant of GaAs.

Bastard's work[2] was followed by papers by Greene and Bajaj,[3] and Mailhiot *et al.*[4] Greene and Bajaj[3] have considered hydrogenic impurity states of a donor atom at the center of a GaAs quantum well of finite depth, sandwiched between two semi-infinite slabs of $Ga_{1-x}Al_xAs$. In their calculations the effective mass and static dielectric constant used were those of GaAs both inside and outside of the GaAs quantum well. These authors have reasoned that this procedure is permissible since the parameters used were such that the donor electron has been largely confined to the GaAs quantum well. In the calculations of Mailhiot *et al.*,[4] who have also considered hydrogenic impurity states, the same assumption was made for the effective mass, but the image charges arising from the dielectric mismatch on the interfaces between the GaAs layer and the two semi-infinite slabs of $Ga_{1-x}Al_xAs$ have also been considered.

In all of the above calculations[2-4] the conduction band of GaAs has been assumed to be parabolic. The effect of the nonparabolicity of the conduction band of GaAs on the hydrogenic donor levels has been recently assessed by Chaudhuri and Bajaj.[5] Finally, in a very recent work, Priester *et al.*[6] have addressed the problem of the binding energies of hydrogenic impurities in finite quantum-well structures with effective-mass mismatch.

The purpose of the present work is to go beyond the hydrogenic approximation by considering the dielectric response of a single GaAs quantum well of infinite depth to the presence of a donor ion. (The infinite-depth assumption is made in order to get away from the complications arising from the effective-mass mismatch associated with a GaAs quantum well of finite depth). This goal is accomplished by making use of the dielectric response theory of Resta.[7] In this theory all calculations can be carried out in ordinary space. The salient feature of Resta's theory[7] is that at a distance R from the donor ion the screening of the charge by the valence electrons of GaAs (considered to form an isotropic and homogeneous electron gas) is complete. This means that for distances larger than R from the charge, the Coulomb interaction

between the donor ion and the donor electron is scaled by the static dielectric constant of GaAs, while for distances less than R from the charge the screening of the charge by the valence electrons of GaAs is incomplete. In the present work, the partial screening of the charge is introduced into the Coulomb term of the Hamiltonian by the spatial dielectric function of GaAs. In our two-stage calculations we have made use of Resta's linearized analytical theory,[7] as well as his nonlinear theory.[7,8] For the latter we have used the analytical approximation of Csavinszky and Brownstein.[9,10]

This paper is organized as follows. In Sec. II A the effect of the linearized dielectric response of GaAs on the ground state of a donor atom is considered. In Sec. II B similar investigations are carried out using the nonlinear dielectric response of GaAs. In Sec. III we compare our results with those of Bastard[2] and analyze our findings, and in Sec. IV we present our conclusions.

We note that all quantities appearing in this paper are expressed in atomic units.[11] We further note that in what follows the subscripts l and n refer to the words linear and nonlinear, respectively.

II. THEORY

A. Application of the linearized screening theory

Neglecting image forces, and assuming a parabolic conduction band associated with a scalar effective mass m^*, the Hamiltonian in circular cylindrical coordinates for a single donor atom placed in a GaAs quantum well is given[2] by

$$\mathscr{H}_l=-\frac{1}{2m^*}\nabla^2-\frac{1}{\bar{\epsilon}_l(r)[\rho^2+(z-z_i)^2]^{1/2}}+V(z)\ . \tag{1}$$

In Eq. (1), z_i is the donor ion position (the z origin is chosen at the center of the well), while $\rho=(x^2+y^2)^{1/2}$ is the distance measured in the GaAs layer parallel to the interfaces (the impurity site is the x and y origin). Also in Eq. (1), $V(z)$ is the potential-energy barrier[12,13] which confines the electron in the well of thickness L, and $\bar{\epsilon}_l(r)$ is the linear spatial dielectric function.[7] These quantities are given by[2]

$$V(z)=\begin{cases}+\infty & \text{for } |z|>L/2\ ,\\ 0 & \text{for } |z|<L/2\ ,\end{cases} \tag{2}$$

and by[7]

$$\bar{\epsilon}_l(r)=\begin{cases}\dfrac{\epsilon(0)qR_l}{\sinh[q(R_l-r)]+qr} & \text{for } r\le R_l\ ,\\ \epsilon(0) & \text{for } r\ge R_l\ .\end{cases} \tag{3}$$

In Eq. (3), $\epsilon(0)$ is the static dielectric constant of GaAs, and q is a constant related to the valence Fermi momentum k_F by[7]

$$q=(4k_F/\pi)^{1/2}\ . \tag{4}$$

Also in Eq. (3), R_l is a screening radius which is determined from[7]

$$\frac{\sinh(qR_l)}{qR_l}=\epsilon(0)\ . \tag{5}$$

Choosing the same ground-state trial wave function as Bastard,[2] namely,

$$\psi=\begin{cases}N\cos(k_1z)\exp\left[-\dfrac{1}{\lambda}[\rho^2+(z-z_i)^2]^{1/2}\right] & \text{for } |z|\le L/2,\\ 0 \text{ for } |z|\ge L/2\end{cases} \tag{6a}$$

with

$$k_1=\pi/L\ , \tag{6b}$$

where N is a normalization constant and λ is a variational parameter, the eigenenergy $e_l(L,z_i)$ of Eq. (1) is obtained from

$$e_l(L,z_i)=\int\psi^*\mathscr{H}_l\psi\,d\tau\ , \tag{7}$$

subject to the requirement

$$\frac{\partial e_l(L,z_i)}{\partial\lambda}=0\ . \tag{8}$$

The binding energy of the donor atom, $E_l(L,z_i)$, is calculated from[2]

$$E_l(L,z_i)=\frac{1}{2m^*}\frac{\pi^2}{L^2}-e_l(L,z_i)\ . \tag{9}$$

The result of our calculations for $z_i=0$, together with Bastard's result[2] that we have recalculated, is presented in Fig. 1. Similar results for $z_i=L/4$, and $L/2-R_l$ are presented in Figs. 2 and 3.

B. Application of the nonlinear screening theory

As shown by Csavinszky and Brownstein,[9,10] on the basis of a variational approach the spatial dielectric function resulting from Resta's nonlinear theory[7,8] is well approximated by

$$\bar{\epsilon}_n(r)=\begin{cases}[K(r)P(r)+M(r)]^{-1} & \text{for } r\le R_n\ ,\\ \epsilon(0) & \text{for } r\ge R_n\end{cases} \tag{10}$$

with

$$K(r)=1+\beta[\exp(-r/\alpha)-1]\ , \tag{11}$$

$$P(r)=\sinh[q(R_n-r)]/\sinh(qR_n)\ , \tag{12}$$

$$M(r)=r/\epsilon(0)R_n\ , \tag{13}$$

where the quantities β, α, and R_n (the screening radius) are variational parameters. Their values, for a charge $Z=+1$ placed into a GaAs quantum well, are given in Table II together with the values of $\epsilon(0)$ and k_F.[14–16]

The Hamiltonian for the present case is

$$\mathscr{H}_n=-\frac{1}{2m^*}\nabla^2-\frac{1}{\bar{\epsilon}_n(r)[\rho^2+(z-z_i)^2]^{1/2}}+V(z)\ , \tag{14}$$

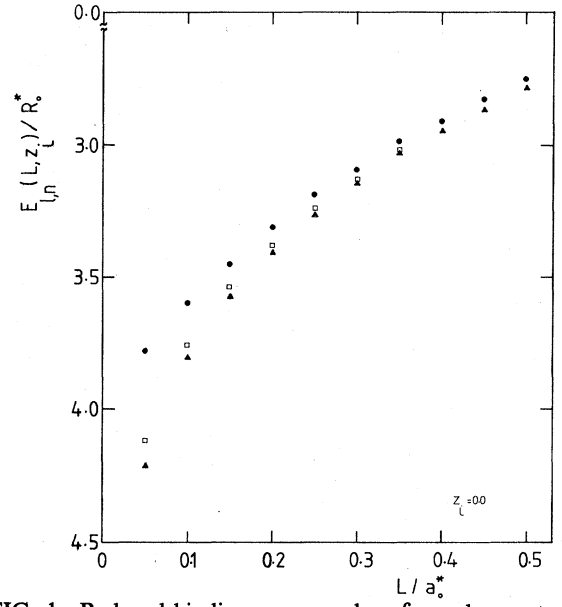

FIG. 1. Reduced binding energy values for a donor atom at $z_i=0$ (●, hydrogenic theory; ▲, linearized screening theory; □, nonlinear screening theory).

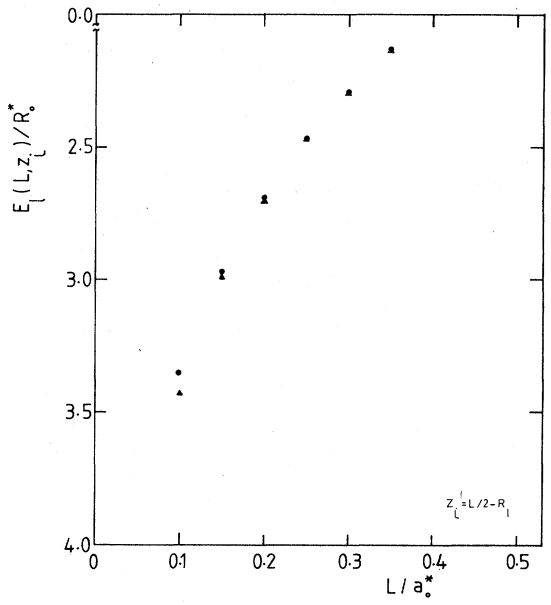

FIG. 3. Reduced binding energy values for a donor atom at $z_i=L/2-R_l$ (●, hydrogenic theory; ▲, linearized screening theory).

and the eigenenergy $e_n(L,z_i)$ and binding energy $E_n(L,z_i)$ are obtained from Eqs. (7)—(9) with the replacement of $\mathscr{K}_l$ in Eq. (7) by $\mathscr{K}_n$. The result of our calculations for $z_i=0$ is presented in Fig. 1.

III. DISCUSSION

Figure 1 shows how the reduced binding energy of a donor atom, located at the center of the well, depends on the width of the well. (a) It is seen from Fig. 1 that, at a given value of L, consideration of the dielectric response of the well leads to an increase in the magnitude of the binding energy relative to the corresponding hydrogenic value. (b) Figure 1 further shows that the discrepancy between our values and the corresponding hydrogenic values is a function of the width of the well, becoming less pronounced as the width of the well is increased. (c) It is also seen from Fig. 1 that, at a given value of L, both the linear and the nonlinear screening theories of Resta[7] predict about the same binding energies. For this reason, in further calculations, we have used only the simpler

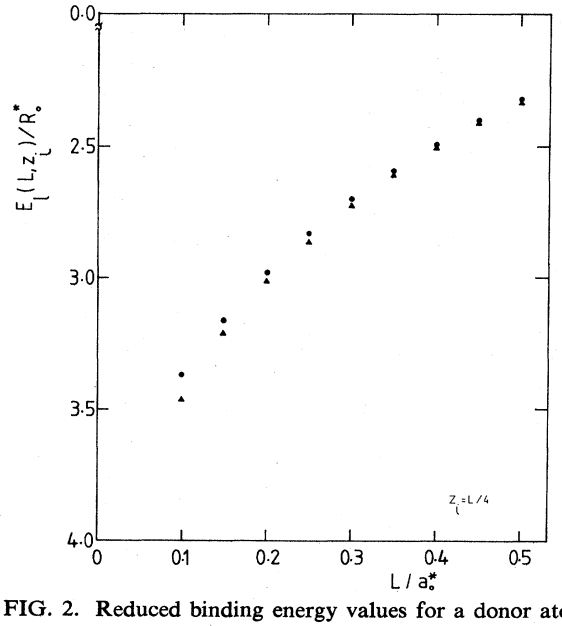

FIG. 2. Reduced binding energy values for a donor atom at $z_i=L/4$ (●, hydrogenic theory; ▲, linearized screening theory).

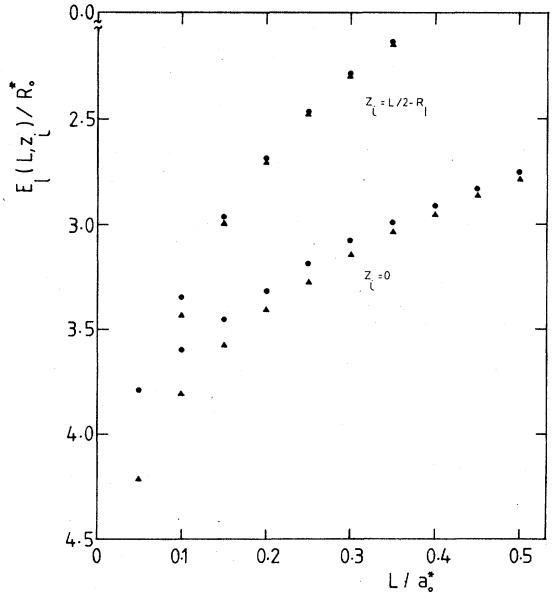

FIG. 4. Reduced binding energy values versus well width for two donor-ion positions.

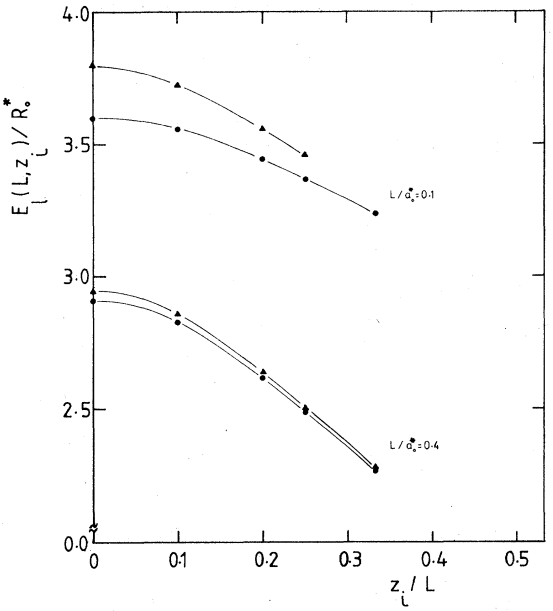

FIG. 5. Reduced binding energy values versus donor-ion position for two well widths.

linear screening theory.

To explain finding (a), we point out that the contribution to the eigenenergy e_l [Eq. (7)], from the second term of $\mathscr{H}_l$ [Eq. (1)] is a negative quantity. We also point out that, in the $0<r<R_l$ region, $\bar{\epsilon}_l(r)<\epsilon(0)$. For this reason, we expect that in the approach based on the use of the linear spatial dielectric function the magnitude of the negative contribution from the second term of $\mathscr{H}_l$ is larger than that furnished by the approach that is based on the use of the static dielectric constant. In view of the fact that the eigenenergy e_l is a positive quantity, the consequence is that the eigenenergy obtained with the use of the spatial dielectric function is less than the eigenenergy obtained by using the static dielectric constant. It follows then that the magnitude of the binding energy E_l [Eq. (9)] is larger when using the spatial dielectric function than that obtained with the use of the static dielectric constant. This then explains why our binding energies at various values of L are larger in magnitude than the hydrogenic binding energies of Bastard.[2]

To close our discussion of Fig. 1, we mention that we have also calculated binding energies for the $L/a_0^*>0.5$ region, up to $L/a_0^*=10$. To save space, these values are not given here. We merely mention that the trend revealed in Fig. 1 continues; the binding energies converge toward the hydrogenic values as the well width is increased.

TABLE I. Values of the variational parameter as a function of z_i for $L/a_0^*=0.5$.

z_i	λ^B	λ
0	131.69	130.41
$L/5$	144.06	143.13
$L/4$	150.82	150.09
$L/3$	164.45	164.05
$L/2-R_l$	185.99	185.95

TABLE II. Values of various parameters used in the present work.

m^*	0.0665
$\epsilon(0)$	12.56
k_F	0.92
R_1	4.43
R_n	4.22
α	0.28
β	0.1679
a_0^*	$\epsilon(0)/m^*$
R_0^*	$m^*/2[\epsilon(0)]^2$

To explain finding (b), we consider that in a narrow well the volume of the sphere of radius R_l, in which the screening takes place, is more important than in a well of large width. The reason is, that "more" of the donor electron is confined to the screening region in a narrow well than in a well of large width. We can see that this is so by looking at illustrative values of the variational parameter λ. At $L/a_0^*=0.1$, for instance, we have $\lambda=99.07$, while at $L/a_0^*=1.0$, we have $\lambda=152.39$. A glance at Eq. (6a) then shows that the wave function is more spread out in the latter case than in the former one. As a result, the importance of the screening region diminishes as the well width is increased. This then explains why the magnitude of the discrepancy between our binding energies and those of Bastard becomes less with increasing well width.

Figure 2 pertains to an off-center impurity located at $z_i=L/4$. This figure shows that at given values of L, our reduced binding energy values now practically coincide with the hydrogenic values.

Figure 3 pertains to an off-center impurity placed at $z_i=L/2-R_l$. For such an impurity the screening radius R_l just touches the wall of the well. This figure shows that at given values of L, our reduced binding energy values are again in practical coincidence with the hydrogenic reduced binding energy values.

It is mentioned here that in the hydrogenic theory it is possible to place a donor ion at the wall, i.e., at $z_i=\pm L/2$. This, however, is not possible in the present case. The reason is that the spatial dielectric function used in our calculations is based on an isotropic and homogeneous electron-gas model. Clearly, for a donor ion located at the wall, the screening of the charge would take place in a hemisphere in the well, instead of a sphere. Such a situation does not belong to the category of isotropic and homogeneous screening.

The last aspect of the calculations that needs discussion is the finding (see Figs. 1–3) that as the donor ion is moved from the center of the well towards the wall of the well, the binding-energy curve calculated with the linear screening theory rises towards the hydrogenic binding energy curve and practically merges with the latter. We believe this finding has its origin in the behavior of the variational parameter. Table I lists the values of the variational parameter for a few donor ion positions associated

both with the linear screening theory (λ) and with the hydrogenic theory (λ^B) for $L/a_0^*=0.5$. It is seen from Table I that, in both theories, the value of the variational parameter increases as the donor ion approaches the wall of the well. This means that, in both theories, the donor-electron cloud is spread out more and more as the ion gets closer to the wall of the well. One might say that, in both theories, the donor-electron cloud expands as the ion is moved from the center of the well towards the wall of the well. This expansion towards the other wall of the well is loosely equivalent to an increasing p-like character of the electron cloud. (Bastard[2] has shown that in the $L\rightarrow\infty$ limit of a donor ion placed at $z_i=L/2$, the wave function becomes p like). Consequently, for a p-like wave function, the screening region is of lesser importance than for an s-like wave function.

We conclude the discussion of the results of our calculations by presenting Figs. 4 and 5. Figure 4 shows reduced binding energy values versus well width for two values of z_i. Figure 5 shows reduced binding energy values versus donor-atom position for two values of L. While Figs. 4 and 5 do not show new results, they illustrate present results from a different angle. To round out our presentation, we list in Table II the values of various parameters used in our calculations.

IV. CONCLUSIONS

We are now ready to present our conclusions.

(1) The dielectric response to a donor ion in a GaAs narrow quantum well of infinite depth is an important factor in the theory of impurity states in the well and leads to important deviations from the hydrogenic theory.[2]

(2) Use of Resta's linearized screening theory,[7] at least for a charge of $Z=+1$, is sufficient. (For charges $Z>+1$, this is less true[17] and in those cases application of the nonlinear screening theory[7–10] might be called for.)

(3) The discrepancy between reduced binding energies calculated from Bastard's hydrogenic theory[2] and from our theory is a function of the width of the well and the position of the donor ion in the well.

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[1]For a review see H. C. Casey and M. B. Panish, *Heterostructure Lasers* (Academic, New York, 1978), Part, A, p. 193.

[2]G. Bastard, Phys. Rev. B **24**, 4714 (1981).

[3]R. L. Greene and K. K. Bajaj, Solid State Commun. **45**, 825 (1983).

[4]C. Mailhiot, Y. C. Chang, and T. C. McGill, Phys. Rev. B **26**, 4449 (1982).

[5]S. Chaudhuri and K. K. Bajaj, Phys. Rev. B **29**, 1803 (1984).

[6]C. Priester, G. Bastard, G. Allan, and M. Lannoe, Phys. Rev. B **30**, 6029 (1984).

[7]R. Resta, Phys. Rev. B **16**, 2727 (1977).

[8]F. Cornolti and R. Resta, Phys. Rev. B **17**, 3239 (1978).

[9]P. Csavinszky and K. R. Brownstein, Phys. Rev. B **24**, 4566 (1981).

[10]P. Csavinszky and K. R. Brownstein, Phys. Rev. B **25**, 1362 (1982).

[11]$m_0=1$, $e_0^2=1$, $\hbar=1$, unit of length a_0 is the bohr, unit of energy e_0^2/a_0 is the hartree.

[12]Equation (1), without the second term on the right-hand side, is the "classical" problem of an electron in a one-dimensional square well.[13]

[13]A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), Vol. 1, Chap. 3.

[14]This quantity is calculated from $k_F=(3\pi^2 n_0)^{1/3}$, where n_0 is the density of the valence electrons. To obtain n_0, one considers that the GaAs unit cube has a cube side of 10.684 a.u. (Ref. 15), and contains four Ga atoms and four As atoms (Ref. 16), with a Ga atom contributing three electrons and an As atom five electrons.

[15]R. W. G. Wyckoff, *Crystal Structures* (Wiley, New York, 1963), Vol. 1, p. 112.

[16]C. Kittel, *Introduction to Solid State Physics*, 5th ed. (Wiley, New York, 1976), p. 26.

[17]P. Csavinszky, Phys. Rev. B **21**, 632 (1980).