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Bound polaron in GaAs-GaAlAs quantum-well structures

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The effects of the electron-phonon interaction on the ground bound state of an isolated hydrogenic impurity in a GaAs-GaAlAs quantum well containing free carriers are calculated as a function of the electron density for different values of the well thickness. The screening effects of the impurity potential and the electron-phonon interaction are described within the random-phase approximation. It was found that the polaronic contribution to the impurity binding energy is quite significant. In the case of thin quantum wells this correction ranges from about 5% at high electronic densities to 10% at low electron concentrations.

The electronic properties of two-dimensional semiconductor structures such as superlattices and multiple-quantum wells have been the subject of increasing interest.[1] The superlattices consisting of alternate layers of GaAs and GaAlAs are the simplest and the most intensively studied heterostructures. The presence of impurities within these systems plays a fundamental role on transport mechanisms at low temperatures. Their associated electronic bounds states are hydrogenlike states similar to those found in the impurity problem in metal-oxide-semiconductor structures.

Though a number of papers[2-5] have appeared in the literature dealing with various aspects of the energy levels of impurities in GaAs-GaAlAs, theoretical understanding of these bound states and their binding energies is still incomplete. Bastard[2] first calculated the ground bound state of a hydrogenic impurity as a function of the layer thickness and of the impurity position inside the well. In his calculation the barrier height of the quantum well was assumed to be infinite at the interfaces. Mailhiot *et al.*[3] and Greene and Bajaj[4] improved his calculation by assuming a finite potential barrier with a hydrogenic impurity in the middle of the well. In a subsequent work, Tanaka *et al.*[5] investigated the case where the impurity could be located outside the GaAs layer, that is the case of modulation doping. In taking into account the effects of screening due to the free electrons confined in the quantum well, Brum *et al.*[6] calculated the binding energy of a single Coulombic impurity as a function of the electron concentration. Recently, Ioriatti and Tsu,[7] by means of a variational procedure which incorporates all the miniband states, calculated the binding energy of an hydrogenic impurity in a GaAs-GaAlAs superlattice. In the limit of large barrier width, their results are similar to those of an isolated quantum well. Although in these works several important aspects of the problem such as finite barrier, impurity screening, etc. have been incorporated in their model calculation, they have neglected the electron interaction with the optical phonons of the GaAs.

In this paper we report the first calculation of the polaronic effects on the ground bound state of an isolated hydrogenic impurity located at the middle or at the barrier of a GaAs-GaAlAs quantum well structure containing free carriers. By using a variational formalism we calculate the binding energies as a function of the free electrons density for several values of the well thickness. In addition, we also obtain the polaronic mass correction versus the electron concentration. The screening effects of the impurity and of the electron-phonon coupling by the free carriers present in the well are described within the random-phase approximation (RPA). We will show that the polaronic effects are quite important, increasing the values of the binding energies significantly.

Let us consider the bound-state problem associated to a single Coulombic impurity located at $z=z_i$ in a GaAs-GaAlAs quantum well of infinite barrier and width L, confining free carriers. We consider the electrons to be interacting with the optical phonons of this semiconductor structure. In the framework of the effective mass approximation the Hamiltonian of this system can be written as

$$H=\frac{\mathbf{p}^2}{2m}+V(z)+V_s(\mathbf{r})+\sum_{\mathbf{q}}\hbar\omega_{L0}a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}} +\sum_{\mathbf{q}}\Gamma_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}(a_{\mathbf{q}}^{\dagger}+a_{-\mathbf{q}}) , \qquad (1)$$

where $\mathbf{p}=(\mathbf{P},p_z)$ and $\mathbf{r}=(\mathbf{R},z)$ are the electron momentum and coordinate, respectively, m is the electron band mass, $V(z)=0$ for $0<z<L$, and $V(z)=+\infty$ otherwise. $V_s(\mathbf{r})$ is the screened Coulombic impurity potential calculated in the RPA. $a_{\mathbf{q}}^{\dagger}$ is the creation operator for the optical phonon of wave vector $\mathbf{q}=(\mathbf{Q},q_z)$ and frequency ω_{L0}, and $\Gamma_{\mathbf{q}}$ is the Fourier coefficient of the screened electron-phonon interaction.

In order to calculate the ground-state energy, we choose a trial wave function as

$$\psi(\mathbf{r})=(2/\pi\lambda^2)^{1/2}\phi(z)\exp(-R/\lambda)U\,|\,0\rangle , \qquad (2)$$

where

$$\phi(z)=(2/L)^{1/2}\sin(\pi z/L) \qquad (2a)$$

is the electron ground-state wave function for an infinite

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well of width L,

$$U=\exp\left[\sum_{\mathbf{q}}(f_{\mathbf{q}}a_{\mathbf{q}}^{\dagger}-f_{\mathbf{q}}^{*}a_{\mathbf{q}})\right] \tag{2b}$$

is a unitary transformation, which displaces the phonon coordinates, and $|0\rangle$ represents the state with no phonons present, i.e., the vacuum state. The variational function $f_{\mathbf{q}}$ and parameter λ are to be determined by minimizing the expectation value of the Hamiltonian H, Eq. (1).

The average of the screened Coulombic impurity $V_s(\mathbf{r})$, analyzed into Fourier components $V_s(\mathbf{Q},z)e^{i\mathbf{Q}\cdot\mathbf{R}}$, is given by

$$\bar{V}_s=\langle\psi\,|\,V_s(\mathbf{r})\,|\,\psi\rangle$$
$$=(2/\pi\lambda^2)\int e^{-2R/\lambda}\bar{V}_s(\mathbf{Q})e^{i\mathbf{Q}\cdot\mathbf{R}}\frac{d\mathbf{Q}}{(2\pi)^2}d\mathbf{R}\ , \tag{3}$$

where

$$\bar{V}_s(\mathbf{Q})=\langle\phi(z)\,|\,V_s(\bar{Q},z)\,|\,\phi(z)\rangle$$
$$=\frac{-2\pi e^2}{\kappa Q\epsilon(\mathbf{Q})}\langle\phi(z)\,|\,e^{-Q|z-z_i|}\,|\,\phi(z)\rangle\ . \tag{4}$$

κ is the lattice dielectric constant of the semiconductor structure, z_i is the position of the impurity in the well, and $\epsilon(\mathbf{Q})$ is the two-dimensional static wave-vector-dependent dielectric function of the electronic system given by[8]

$$\epsilon(\mathbf{Q})=1+(2/a_0^*Q)G(\mathbf{Q})F(\mathbf{Q})\ , \tag{5}$$

with $a_0^*=\kappa\hbar^2/me^2$ being the effective Bohr radius. $G(\mathbf{Q})$ is a function which takes into account the size of the Fermi surface in the following form:

$$G(\mathbf{Q})=\begin{cases}1, & Q<2Q_F\\ 1-[1-(2Q_F/Q)^2]^{1/2}, & Q>2Q_F\ .\end{cases} \tag{6}$$

The screening form factor $F(\mathbf{Q})$ associated with the quasi-two-dimensional confinement of the electrons is defined as[8]

$$F(\mathbf{Q})=\int dz\,dz'\ |\phi(z)|^2e^{-Q|z-z'|}|\phi(z')|^2\ , \tag{7}$$

which for the infinite barrier of the quantum well turns out to be

$$F(x)=\frac{2(x^2+8\pi^2)}{(x^2+4\pi^2)^2}(1-e^{-x})+\frac{x}{x^2+4\pi^2}$$
$$+\frac{2}{x}\left[1-\frac{1}{x}(1-e^{-x})\right]\ ,\quad x\equiv QL\ . \tag{8}$$

In the case of a purely two-dimensional system, $L\to0$ and $F(Q)\to1$.

Let us consider now the polaronic contribution to the binding energy. Since the dimensionless Fröhlich coupling constant α which characterizes the electron-phonon potential strength is small for GaAs ($\alpha=0.06$), the calculation of the polaronic energy and mass correction can be straightforwardly performed by using the Lee, Low, and Pines variational method.[9]

In taking into account the electron-phonon interaction screened by the static dielectric function in the random-phase-approximation and the usual form factor associated with the two-dimensional carrier confinement, the polaronic energy shift E_p and effective mass correction $\Delta m=(m_p-m)/m$, where m_p and m are the polaron and band mass respectively, are given by[9]

$$E_p=-64\alpha\hbar\omega_{LO}\int_0^{\infty}dx\frac{F(x)}{(1+\lambda^2x^2/r_p^2)^3[\epsilon(x)]^2} \tag{9}$$

and

$$\Delta m=128\alpha\int_0^{\infty}dx\frac{x^2F(x)}{(1+\lambda^2x^2/r_p^2)^3[\epsilon(x)]^2}\ , \tag{10}$$

where r_p is the polaron radius. The variational ground-state energy $E=\langle\psi\,|\,H\,|\,\psi\rangle$ has then the following form,

$$E=\frac{\hbar^2}{2m}\left[\frac{1}{4\lambda^2}+\frac{\pi^2}{L^2}\right]+\bar{V}_s+E_p\ , \tag{11}$$

with $\bar{V}_s$ and E_p given by Eqs. (3) and (9), respectively. Minimizing E with respect to the parameter λ leads to the ground-state energy of the system. The difference between this value and the lowest E for the system without the impurity gives the ground-state binding energy of the donor impurity.

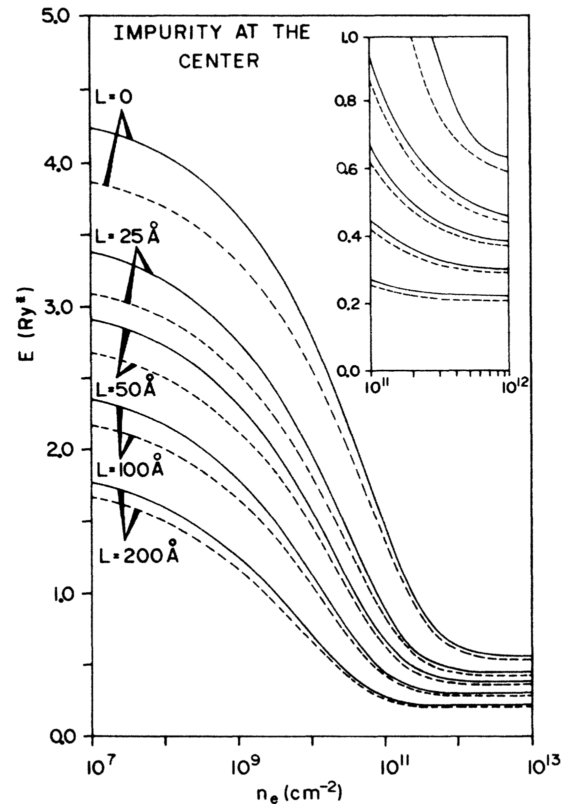

FIG. 1. Binding energy of a screened hydrogenic impurity located at the center of a GaAs-GaAlAs quantum well containing free electrons as a function of the electronic density n_e for different values of the well thickness. The solid and dashed curves correspond to the case with and without the electron-phonon interaction. The curves labeled $L=0$ represent an ideally two-dimensional electron gas. The insets show an amplification of the binding energy in the high electronic concentration region.

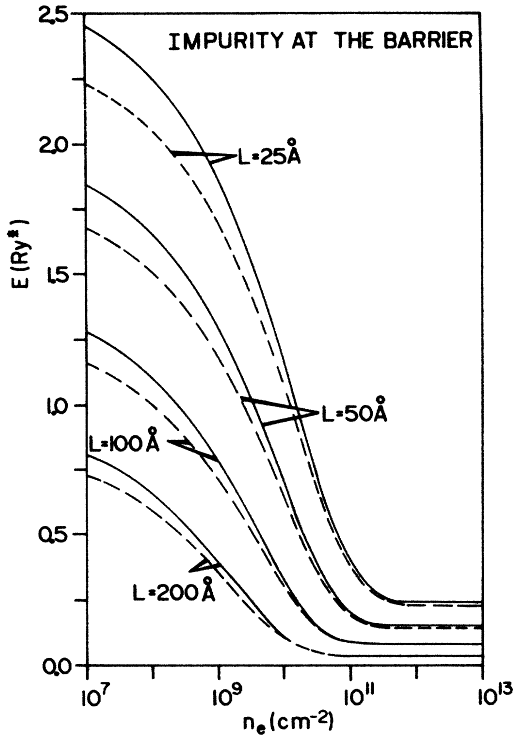

FIG. 2. Binding energy of an impurity placed at the boundary of the barrier of a doped GaAs-GaAlAs quantum well versus the carrier concentration n_e for different layer thickness. The solid and dashed curves represent the system with and without the electron-phonon coupling.

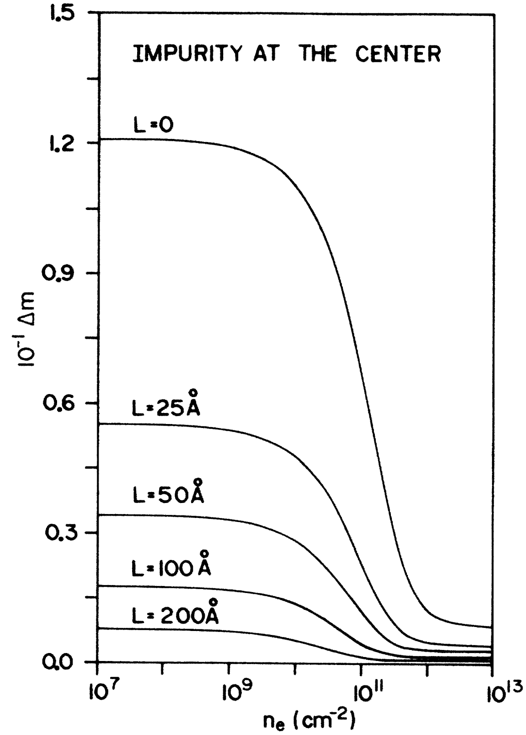

FIG. 3. Polaronic mass correction $\Delta_m = (m_p - m)/m$, where m and m_p are the band and polaron masses, respectively, as a function of the electron density n_e in a GaAs-GaAlAs quantum well with a screened impurity placed at the center of the well. Four different values of the layer thickness and the ideally two-dimensional system are considered.

The results we have obtained by numerically minimizing the energy expression Eq. (9), with and without the electron-phonon interaction for several values of the width of the quantum well are shown in Figs. 1 and 2. The binding energy is plotted as a function of the two-dimensional electron concentration for two different positions of the impurity in the GaAs layer namely at the center of the well (Fig. 1) and at the boundary of the barrier (Fig. 2). The percentual shifts of the donor-level binding energy due to the polaronic effects for different layer thickness L and several electronic densities n_e are also shown in Table I. As we can see, for a given well thickness the polaronic correction to the binding energy increases with decreasing the electron concentration. We also can note that for a given n_e the polaronic contribution is larger for smaller well thickness. Then, the largest contribution comes from the purely two-dimensional situation ($L=0$) and ranges from about 5.5% at high electronic densities ($n_e \simeq 10^{12}$ cm^{-2}) to more than 10% in the low-density regime ($n_e \rightarrow 0$).

In each separate case, where the impurity is located, or at the center or at the boundary of the barrier of the quantum well, the importance of the electron-phonon is much more pronounced as the binding energy becomes larger. Then in a quantum well with finite barrier height where the binding energies are smaller than ours the polaronic effects will be a little weaker.

From the results of Table I one notices that for a given well thickness and low carrier concentration, the shift of the binding energy due to the electron-phonon coupling is

TABLE I. Percentual shifts of the binding energy $\Delta E_B = [(E_B^* - E_B)/E_B] \times 100$, where E_B^* and E_B are the binding energies with and without the electron-phonon coupling, respectively, for different values of the layer thickness L and several values of the electronic density n_e. The impurity is located at the boundary of the barrier B or at the center C of the quantum well.

L (Å) \ n_e (cm^{-2})	10^7		10^8		10^9		10^{10}		10^{11}		10^{12}	
Impurity position	B	C	B	C	B	C	B	C	B	C	B	C
0	9.7	9.7	9.7	9.7	9.6	9.6	9.3	9.3	8.2	8.2	5.5	5.5
25	9.8	9.2	9.7	9.1	9.5	8.9	8.9	8.5	5.9	6.8	3.9	4.7
50	9.9	8.9	9.8	8.8	9.6	8.6	8.8	8.0	4.6	6.0	3.5	4.3
100	10.3	8.6	10.2	8.3	9.9	8.1	8.6	7.4	3.3	5.0	2.2	3.9

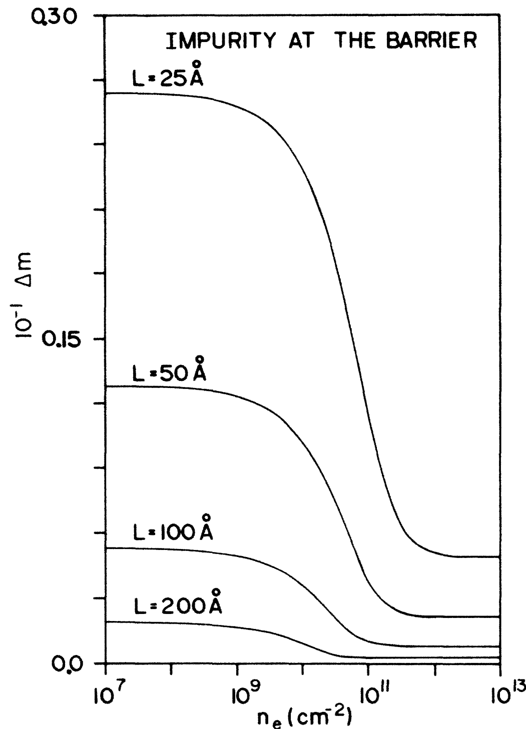

FIG. 4. Same as Fig. 3 but with the screened impurity located at the boundary of the barrier of the quantum well.

larger when the impurity is placed at the boundary of the barrier. On the other hand, at high electron density this situation is reversed and the polaronic contribution becomes larger in the case where the impurity is located at the middle of the quantum well. These results make explicit the fact that screening effects play a fundamental role. As the screening increases by increasing the electron concentration, the spatial extension of the impurity wave function in the plane of the layer becomes larger and this in turn increases the importance of the electron-phonon coupling.

In Figs. 3 and 4 we show the polaronic mass correction $\Delta m = (m_p - m)/m$, where m_p and m are the polaron and band masses, respectively, as a function of the free carrier concentration n_e, for several values of the GaAs layer thickness and for two different positions of the impurity in the quantum well. In both cases where the impurity is placed at the center or at the boundary of the barrier, the results are qualitatively similar. For a given layer thickness, the polaronic mass correction is almost n_e independent at low electronic density ($n_e < 10^{10}$ cm^{-2}), decreases with increasing n_e, and reaches a saturation value at high carrier concentration ($n_e > 10^{12}$ cm^{-2}). Note that this saturation value becomes smaller as the layer thickness increases. One should also notice that by increasing the well thickness, the three-dimensional results, where either the binding energy of a screened impurity as the polaronic mass correction vanishes, are restored at high electron concentration. When the impurity is placed at the center of the quantum well, the localization of the electron becomes more pronounced and as a consequence the polaronic mass correction becomes larger as compared to the case where the impurity is located at the barrier.

In conclusion, we have calculated for the first time the effects of electron-phonon interaction in the binding energy of a single hydrogenic impurity placed or at the middle or at the boundary of the barrier of a doped GaAs-GaAlAs quantum well. The random-phase-approximation has been used to describe the screening effects for both the impurity potential and the electron-phonon interaction. Our calculations show a significative correction to the impurity binding energy due to the polaronic effects. Finally, the results explicitly show the quantitative importance of the screening effects which play a fundamental role in the understanding of this problem.

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[1]*Proceedings of the 17th International Conference on the Physics of Semiconductors, San Fransciso, 1984*, edited by J. D. Chadi and W. A. Harrison (Springer-Verlag, New York, 1984).

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