Screening effects in modulation-doped quantum wells

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The ground bound state of a hydrogenic impurity, screened by the free carriers of a modulation-doped quantum well, is investigated. The dielectric function is calculated at finite temperature in the random-phase approximation and the impurity is located either in the well or in the barrier. Temperature influence on the binding energy is noticeable for low carrier density ($n_e \sim 10^{11}/\text{cm}^2$) quantum wells. The binding energy of impurities located at the interfaces is strongly temperature dependent because of the screening associated with their own excited carriers.

INTRODUCTION

The screening behavior of a quasi-two-dimensional electron gas (2D EG) has attracted considerable attention in the past, mainly due to the existence of quasi-two-dimensional systems such as inversion layers. Besides, a good knowledge of the screening effect is essential for the understanding of many properties of the 2D EG. The polarizability of a 2D EG was calculated by Stern[1] by considering the two-dimensional analog of the Lindhard dielectric constant while the Thomas-Fermi screening parameter was used in the study of inversion layers.[2,3] Effects of finite temperature[4] and level broadening due to ionized impurities[5–8] have been more recently introduced in the screening dielectric function.

The presence of charged impurities located within the 2D EG determines, in part, transport properties at low temperature and may lead to localized states. Screening of these impurities by the 2D EG plays a fundamental role which can be studied through the bound states associated with a hydrogenic impurity since the binding energies are thought to greatly depend on the free-carrier density.[2,3] Until recently,[9] most of the studies related to bound states associated with a screened impurity were concerned with the metal-oxide-semiconductor (MOS) system. However, for electrons trapped in the quantum wells of a semiconductor superlattice, the structural parameters such as the barrier height or well width are well controlled. Moreover, the free-carrier density and well thickness can be varied as independent parameters. Both are known to strongly influence the binding energy of an impurity.[2,3,10] Finally, impurities can be placed either in the well or in the barrier in a controlled manner.

The main purpose of this paper is to investigate the effects of electronic screening on the ground bound state of an isolated hydrogenic impurity in a quantum well. By using two variational wave functions associated with the first subband of a modulation-doped quantum well, we calculate the binding energy versus the free-carrier concentration. We study the dependence of the impurity state on the impurity site. Finally, we also investigate the effect of finite temperature on the binding energy. It is expected to be related to the temperature dependence of mobility in modulation-doped quantum wells.

GROUND SUBBAND OF A MODULATION-DOPED QUANTUM WELL

We consider first a quantum well of width L and barrier height V_w. n_e is the two-dimension electron gas density. In the following we assume a constant effective mass m^* and a uniform background dielectric constant K through the whole structure. This is a good approximation for the GaAs $Ga_{1-x}Al_xAs$ quantum well which will be considered hereafter. Then in the Hartree approximation, the electronic Hamiltonian for a quantum well free of impurity is given by

$$\mathscr{H}_0=\mathscr{H}_{\text{sq}}+V_e(z) \tag{1}$$

with

$$\mathscr{H}_{\text{sq}}=p^2/2m^*+V_w(z)\ ,$$

where $V_w(z)$ is the square-well potential. If the well center is taken as the z origin, we have

$$V_w(z)=V_wH(\,|z|-L/2)\ , \tag{2}$$

where H is the Heaviside step function.

The eigenfunctions and the eigenvalues of $\mathscr{H}_{\text{sq}}$ are well known; the even bound states are

$$i=0,2,4,\ldots,$$
$$\chi_i^{\text{sq}}(z)=A\cos(kz),\quad |z|<L/2\ ,$$
$$\chi_i^{\text{sq}}(z)=B\exp[-K_i(z-L/2)]\ ,\quad z>L/2\ ,$$
$$\chi_i^{\text{sq}}(-z)=\chi_i^{\text{sq}}(z)\ , \tag{3}$$

and

$$E_i^{\text{sq}}=\hbar^2k_i^2/2m^*\ ,$$
$$E_i^{\text{sq}}=V_w-\hbar^2K_i^2/2m^*\ ,$$
$$k_i\tan(k_iL/2)=K_i\ .$$

$V_e(z)$ is the Hartree potential due to the free-carrier charge. It should be solved self-consistently with $\mathscr{H}_0$. However, for sufficiently thin quantum wells ($L \lesssim 300$ Å) and if the ground subband is the only one populated, this band bending is given with good accuracy[11] by the following Poisson equation:

$$\frac{d^2V_e}{dz^2}=e^2[\chi_0^{sq}(z)]^2/\epsilon_0 K \ . \tag{4}$$

$V_e(z)$ is even and couples the even eigenfunctions χ_i^{sq} of the square well. In the restricted basis $(|\chi_0^{sq}\rangle, |\chi_2^{sq}\rangle)$, we solve the Schrödinger equation for $\mathscr{H}_0$. The ground eigenenergy E_0 is the solution of

$$\begin{vmatrix} E_0^{sq}+V_{00}-E_0 & V_{02}, \\ V_{20}, & E_s^{sq}+V_{22}-E_0 \end{vmatrix}=0 \ , \tag{5}$$

where

$$V_{ij}=\langle\chi_i^{sq}|V_e|\chi_j^{sq}\rangle \ ,$$

and the ground eigenstate is

$$\chi_0=c_0\chi_0^{sq}+c_2\chi_2^{sq}$$

with

$$c_2=c_0\frac{E_0-(E_0^{sq}+V_{00})}{V_{02}} \ ,$$

$$c_0^2+c_2^2=1 \ .$$

If the second excited bound state χ_2^{sq} does not exist, we apply the first-order nondegenerate perturbation V_e on E_0^{sq}:

$$\begin{aligned} E_0&=E_0^{sq}+\langle\chi_0^{sq}|V_e|\chi_0^{sq}\rangle \ , \\ \chi_0&=\chi_0^{sq} \ . \end{aligned} \tag{6}$$

In all of the following, we assume that electrons occupy the ground subband. The chemical potential μ at the temperature T is

$$\mu=E_0+k_BT\ln\left[\exp\left[\frac{\mu_{k_BT=0}}{k_BT}\right]-1\right] \ , \tag{7}$$

with

$$\mu_{k_BT=0}=\pi\hbar^2n_e/m^* \ .$$

SCREENED HYDROGENIC POTENTIAL

We now consider a hydrogenic impurity located at z_i. Because of the presence of the free carrier, this impurity is screened. Carriers redistribute themselves, their density increasing (decreasing) around an attractive (repulsive) potential. The screening behavior of a 2D EG has been described in several ways. One of the most simple is the Thomas-Fermi long-wavelength approximation which gives the screening constant in the electrical quantum limit,[2]

$$s=e^2m^*/2\pi\hbar^2\epsilon_0 K=2/a_0 \ , \tag{8}$$

where a_0 is the bulk Bohr radius.

However, the calculation of bound states is concerned with the response to short wavelength potentials and the Thomas-Fermi approach is likely to overestimate the screening effect in such structures. Moreover, as the screening parameter s is independent of the free-carrier concentration in the electrical quantum limit, the Thomas-Fermi is unable to describe the transition from an unscreened potential to a screened one.

The random-phase approximation (RPA) is a linear self-consistent Hartree approximation. Nonlinear screening has been shown[12] to give better agreement with experimental results for inversion layers in MOS devices. As in two dimensions, any attractive potential is thought to have a bound state, a charged impurity, even after being screened, can have a bound state. In that case, linear screening might be no longer valid.[13] However, if the binding energy is weak, as we expect, it should be a reasonable approximation.

From linear-response theory, if the first subband is the only one considered, the screened potential is a solution of

$$V_i^s(\mathbf{q},z)+\frac{e^2}{\epsilon_0 Kq}\int dz'\chi_0^2(z')e^{-q|z-z'|}\int dz''\chi_0^2(z'')V_i^s(\mathbf{q},z'')\Pi_{\mathrm{RPA}}(q)=V_i(\mathbf{q},z) \ , \tag{9}$$

$V_i^s(q,z)$ and $V_i(q,z)$ are Fourier transforms of the screened and unscreened potentials,

$$\begin{aligned} V_i(q,z)&=\frac{1}{2\pi}\int\int d_r^2e^{-i\mathbf{q}\cdot\mathbf{r}}V_i(\mathbf{r},z) \\ &=-\frac{e^2}{4\pi\epsilon_0 Kq}e^{-q|z-z_i|} \ , \end{aligned} \tag{10}$$

and Π_{RPA} is the RPA polarizability and is calculated at finite temperature, using Maldague's method.

$$\Pi(q,T;\mu)=\int_0^{+\infty}dx\frac{\Pi(\mathbf{q},0;x)}{4k_BT\cosh^2[(\mu-x)/2k_BT]} \ ,$$

with

$$\Pi(q,0;x)=\begin{cases}\dfrac{\epsilon_0 K}{e^2}s, & q\le 2x, \\ \dfrac{\epsilon_0 K}{e^2}s\left[1-\left[\dfrac{4k_x^2}{q^2}\right]^{1/2}\right], & q\ge 2x \ , \end{cases} \tag{11}$$

where

$$s=2/a_0, \quad x=\hbar^2k_x^2/2m^* \ .$$

Averaging (9) over z with $\chi_0^2(z)$, we obtain

$$V_i^s(q)=V_i(q)/\epsilon_{\mathrm{RPA}}(q) \ . \tag{12}$$

$\epsilon_{\mathrm{RPA}}(q)$ is the RPA dielectric function

$$\epsilon_{\mathrm{RPA}}(q)=1+f(q)\frac{e^2}{\epsilon_0 Kq}\Pi_{\mathrm{RPA}}(q) \ . \tag{13}$$

$f(q)$ is a form factor taking into account the finite extension of the function $\chi_0^2(z)$.[9] From (9) and (12) we have

$$\begin{aligned} V_i^s(q,z)=-\frac{e^2}{4\pi\epsilon_0 Kq}\{&e^{-q|z-z_i|}+[1/\epsilon_{\mathrm{RPA}}(q)-1] \\ &\times[g(q,z_i)/f(q)]g(q,z)\} \end{aligned} \tag{14}$$

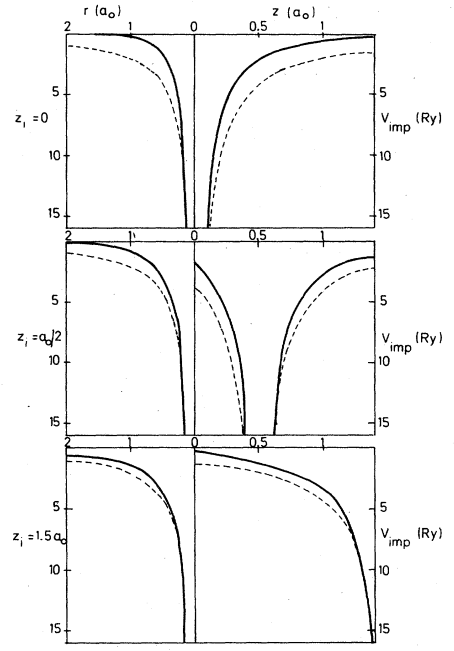

FIG. 1. Screened and unscreened hydrogenic potentials, for a free-carrier density $n_e(\simeq 2.5\times 10^{11}/\mathrm{cm}^2)$ and a well thickness $(=a_0)$ are shown for three different impurity positions: $z_i=0$; $z_i=a_0/2$; $z_i=1.5a_0$. Solid curve, screened potential; dashed curve, unscreened potential. The z dependence is at $r=0$ and the r dependence is at $z=z_i$. The material parameters are $V_w=0.25$ eV, $m^*=0.067m_0$, $a_0=103$ Å, $T=0$ K.

The screening potential is

$$V_i^{\mathrm{SC}}=\frac{-e^2}{4\pi\epsilon_0 K_q}\left[\frac{1}{\epsilon_{\mathrm{RPA}}(q)}-1\right][g(q,z_i)/f(q)]g(q,z)\ . \quad (15)$$

As usual,[14] $e(1/\epsilon_{\mathrm{RPA}}-1)$ is the screening charge. We note that the screening potential is even with respect to z, as it should be, since we do not allow for any excitation in this direction. This parity reflects the parity of the ground state of the quantum well.

$g(q,z_i)$ is the Hartree potential undergone by the impurity located at z_i while $g(q,z)$ is the Hartree potential at z due to the screening charge whose density is given by $e/4\pi\epsilon_0 Kq(1/\epsilon_{\mathrm{RPA}}-1)\,\chi_0^2(z)$.

From Fig. 1, it can be observed that screening in the z direction is important even if it is not as large as in the plane. Screening decreases as the impurity is moved away from the well, due to the rapid drop of χ_0^2.

BINDING ENERGY

The single-impurity problem is described by the Hamiltonian

$$\mathscr{H}=\mathscr{H}_0+V_i^s(r,z)=\mathscr{H}_0+V_i(r,z)+V_i^{\mathrm{sc}}(r,z)\ , \quad (16)$$

where $V_i^{\mathrm{sc}}(r,z)$ is the Hartree potential taking into account the collective redistribution of the free carriers, treated in the random-phase approximation.

The ground state of this Hamiltonian and its binding energy are searched using variational wave functions. The binding energy is defined with respect to the ground subband by

$$E_B=\langle\psi_v\,|\,\mathscr{H}\,|\,\psi_v\rangle-E_0\ , \quad (17)$$

where ψ_v is the variational wave function. Strictly, E_B is not the binding energy since we neglect the influence of bound electrons over electrons contributing to screening.[13] We are likely to overestimate effects of screening because orthogonalization of localized states with extended states is not taken into account. However, localized states are essentially concerned with the extended states of the bottom of the subband $(k<1/a_0)$ where screening is mainly the fact of extended states lying near the Fermi circle. Consequently our approximation may not be too crude for $n_e\gtrsim 10^{11}/\mathrm{cm}^2$.

Two variational wave functions have been tested, both related to the quantum-well ground state. The first one, still used in (9), is

$$\psi_1(r,z)=N_1\chi_0(z)\exp(-r/\lambda_1)\ , \quad (18)$$

where λ_1 is the variational parameter, and N_1 is a normalization coefficient.

In this trial wave function, z and r are separable variables. Consequently the z dependence of the screened potential is of no use since

$$\langle\psi_1\,|\,V_i^s\,|\,\psi_1\rangle=N_1^2\int\int d^2r\exp(-2r/\lambda_1)\times\int dz\,\chi_0^2(z)V_i^2(r,z)$$

or (19)

$$\langle\psi_1\,|\,V_i^s\,|\,\psi_1\rangle=\sum_{\mathbf{q}}V_i^s(q)\int\int d^2r\exp(-2r/\lambda_1)\times e^{i\mathbf{q}\cdot\mathbf{r}}N_1^2\ .$$

In this case, the z_i dependence of the binding energy is

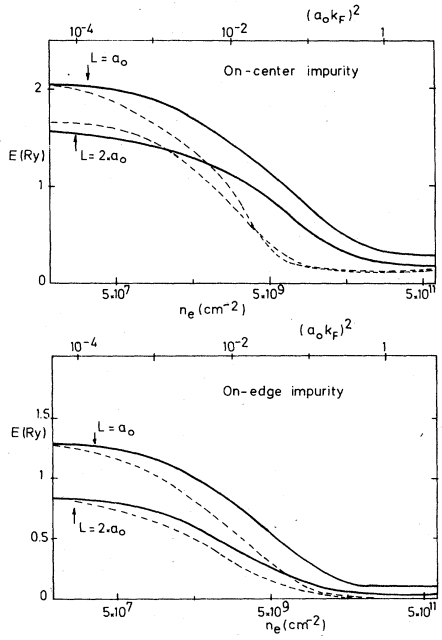

FIG. 2. Binding energy of a screened hydrogenic donor impurity located at the center and at the edge of a GaAs quantum well is plotted versus free-carrier concentration for two well thicknesses: $L=100$ and 200 Å; solid curve, first trial wave function ψ_1; dashed curve, second trial wave function $\psi_2 T=0$ K.

entirely due to the impurity-screened potential itself.

The second trial wave function is

$$\psi_2(\mathbf{r},z)=N_2\chi_0(z)\exp[-\mathbf{q}\cdot\mathbf{r}+(z-z_i)^2/\lambda_2] . \quad (20)$$

The variables r and z are no longer separable. In (20), N_2 is a normalization constant and λ_2 is the variational parameter.

This trial wave function has been shown[10] to be adapted to the impurity problem in the absence of screening. However, it requires a full knowledge of the impurity-screened potential. The n_e dependence of the binding energy, for $T=0$ K, is illustrated in Fig. 2 for two values of L/a_0 and two impurity positions. The energy is expressed in units of Ry, the three-dimensional effective rydberg.

Except in the low n_e region, ψ_1 gives rise to larger binding energies than ψ_2. This is due to the strength of the square-well potential as compared to the screened impurity potential. The z part of the wave function is essentially insensitive to the impurity potential. Subsequently, ψ_1 will be used.

Figure 3 shows the binding energy as a function of the impurity position. It quickly decreases as the impurity moves away from the center of the well. The unscreened impurity binding energies behave similarly[15] but are one order of magnitude greater, indicating that screening does play an important role far in the barrier. Values, for a screened impurity located in the barrier, are comparable to what was calculated in silicon inversion layers.[8] The small binding energies and the large in-plane spreading of their associated wave functions imply a rapid merging of the bound states with the bottom of the ground subband for actual impurity concentrations.

The temperature dependence of the binding energy is illustrated in Figs. 3 and 4. The temperature has little influence on the binding energy for large-enough free-carrier concentration ($n_e \gtrsim 3\times10^{11}/\text{cm}^2$). Screening is then saturated to the Thomas-Fermi limit. At 70 K, k_BT is about one Ry. On the other hand, for $n_e\sim5\times10^{11}/\text{cm}^2$, the Fermi level μ is ~3 Ry and $k_BT<\mu$. The temperature dependence of the binding energy for low n_e ($n_e\simeq10^{11}/\text{cm}^2$) is shown in Fig. 4. One sees that the binding energies associated with impurities located in the well strongly increase with temperature while those of impurities located far in the barrier are rather insensitive to temperature due to weaker screening.

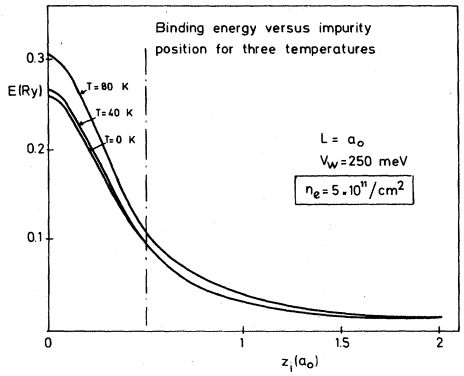

FIG. 3. Binding energy of a screened hydrogenic donor is plotted versus the impurity position for $n_e\simeq5\times10^{11}/\text{cm}^2$ and three different temperatures. $T=0$, 40, and 80 K; $L=a_0$.

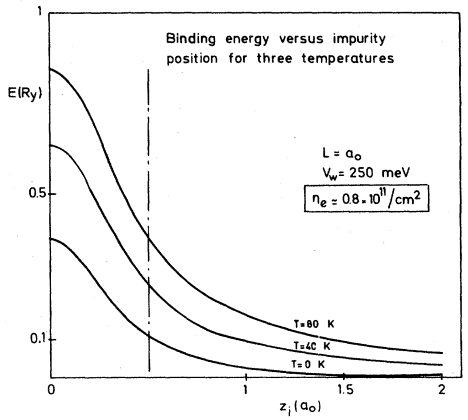

FIG. 4. Binding energy of a screened hydrogenic donor is plotted versus the impurity position for $n_e\simeq0.8\times10^{11}/\text{cm}^2$ and three different temperatures; $T=0$, 40, and 80 K; $L=a_0$.

From extrinsic luminescence experiments,[16,17] it can be thought that some impurities, namely, carbon, are located at one of the quantum-well interfaces. Temperature dependence of the mobility, for low carrier concentration ($n_e\simeq10^{11}/\text{cm}^2$) quantum wells, should be sensitive to the presence of carbon and should allow it to be distinguished from donors in the barrier.

Finally, to illustrate the crucial importance of screening in two-dimensional systems we have calculated the binding energy of impurities screened by their own excited carriers as the temperature is raised. We consider $0.8\times10^{11}/\text{cm}^2$ donors (Si) located at the interfaces of a quantum well. The mean distance between donors (~400 Å) should give an isolated impurity behavior. At

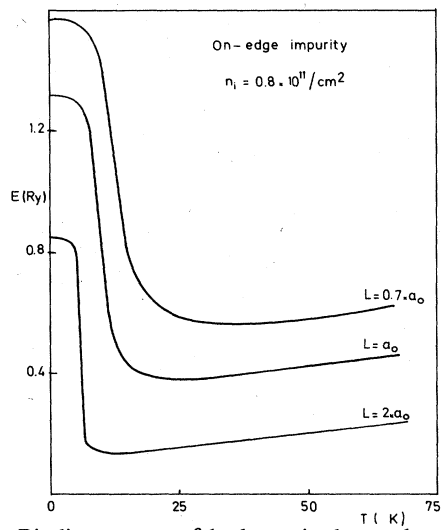

FIG. 5. Binding energy of hydrogenic donors located at the interfaces of a quantum well and screened by excited free carriers is plotted versus temperature for three different well thicknesses: $L=70$, 100, and 200 Å. Hydrogenic donors concentration $n_i=0.8\times10^{11}/\text{cm}^2$.

low temperature, few carriers are excited from their parent donors; their density is governed by the unscreened impurity binding energy. As the temperature goes higher, the ionized impurity number increases as their parent electrons provide screening of the impurities whose binding energy is lowered. Free-carrier density is governed by the impurity binding energy which is influenced by the free-carrier concentration, due to screening. Figure 5 shows the rapid drop of the binding energy with temperature. This drop can be characterized by its temperature for different well widths. At high temperatures, the binding energy slowly increases because of the weakening of screening with temperature and because most of the impurities are ionized.

We have not considered the quasicontinuum of excited bound states,[18,19] energy levels covering a range of energies ΔE below the conduction band, and the scattering on ionized impurities of the Bloch waves. Impurity band and level broadening must be considered in the low-energy side of the density of extended states. However, these points should not strongly modify the binding-energy behavior for donors located at the interfaces but only push it to higher temperatures. On the contrary, level broadening and impurity-band effects cannot be ignored for on center impurities. This point will be further investigated.

CONCLUSION

In conclusion we have investigated the effects of free-carrier screening on the binding energy of a single hydrogenic impurity located in a modulation-doped quantum well. The tested variational wave functions indicate that these effects are quite considerable and that the well potential is predominant as compared to the screened impurity potential. The dependence of the binding energy on temperature suggests mobility experiments with low carrier concentration quantum wells, while screening of donors located at the interfaces by their own excited electrons strongly affect their binding energy as the temperature is varied. Finally, our linear approach of screening still remains tentative and the level broadening effect on the dielectric function requires further investigations.

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