Direct evidence for screening of the Coulomb interaction in quasi-two-dimensional systems

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Magnetic freeze-out of inversion electrons into bound Si donors in GaAs-$Ga_{1-x}Al_xAs$ heterostructures with a spacer has been investigated experimentally and compared with the theory. An inclusion of screening of the Coulomb interaction between electrons and donors is essential for the description of magneto-donor behavior. Features related to overlap of the donor wave functions and the resulting metal-nonmetal transition are demonstrated and discussed.

Behavior of impurities in quasi-two-dimensional (Q2D) structures has attracted in recent years considerable interest due both to its fundamental aspects and importance for applications. In particular, it has been demonstrated experimentally by McCombe and co-workers[1,2] and theoretically by Greene and Bajaj[3] that magneto-optical investigation of magneto-impurities in quantum wells can be used to study the effects of the well confinement on impurity behavior and to characterize selective doping of heterostructures. As in the case of bulk magneto-impurities, the involved physical considerations are directly applicable to hydrogen atoms in gigantic magnetic fields.[4]

It has been recently demonstrated with the use of magneto-transport techniques that one can observe bound magneto-donor states in Q2D structures, in which the impurity atom (a Si donor in $Ga_{1-x}Al_xAs$) is separated from the inversion electron (in GaAs) by a spacer (undoped layer of $Ga_{1-x}Al_xAs$).[5] The magnetic freeze-out of inversion electrons into bound magneto-donor states is observed for not too high spacer values (up to 400 Å) in the ultraquantum limit, in which the inversion electrons occupy only the lowest Landau level. This in turn requires high magnetic fields B and low electron densities N_s. The latter have been reached using the hydrostatic pressure in a procedure described before.[6]

Binding energies of magneto donors have been determined from the temperature dependences of the surface electron density $N_s(T)$ at different magnetic fields in the freeze-out regime. When measuring N_s it is of importance to use all components of the conductivity tensor σ_{xy}.[5,7] At low magnetic fields the structures exhibit metallictype behavior with unactivated electron densities.

The experimental values of magneto-donor binding energies for four different intentionally doped $Ga_{1-x}Al_xAs$-GaAs heterostructures with a spacer are shown in Fig. 1. The essential feature of the data is that the binding energies decrease with increasing spacer widths, indicating that we deal with the states related to Si donors across the spacer.

In Fig. 2 we show the activation energies of magneto donors in sample 3, measured at the same pressure, for which N_s has been varied by changing the speed of cooling of the sample. Since in this case one deals with the same spacer width, it is seen that the activation energy increases with decreasing N_s, or some other quantity related to it.

In their first report Robert *et al.*[5] advanced a semiclassical model, which qualitatively explained the observed phenomena. The basic idea is that the presence of a transverse magnetic field shrinks the donor orbit in the plane parallel to the interface. As a consequence, the electron is on average closer to the donor ion than in the case of $B=0$ and the Coulomb binding energy increases. A characteristic Q2D feature of the situation is related to the interface, which prevents the electron from coming close to the donor as B increases (which is the case in the bulk, cf. Ref. 8). As a result the binding energy should reach a saturation at high fields, its value being determined by the spacer width.

The characteristic parameter for the problem is $\gamma=\hbar\omega_c/2$ Ry*, where $\omega_c=eB/m^*$ is the cyclotron frequency and Ry* is the effective Rydberg. In the theoretical description of magneto-donor states we use the variational procedure, since γ for GaAs and available magnetic fields is in the intermediate range: $0<\gamma<3$. For the donor ground state we take the trial function (cylindrical coordinates) $F(\rho,z)=\varphi(\rho)f(z)$, in which the transverse motion (parallel to the interface) is described by a product of atomictype and magnetictype two-parameter functions: $\varphi(\rho)=A\exp(-\alpha\rho-\beta\rho^2)$, while the longitudinal motion is described by $f(z)=Cz\exp(-b_0z/2)$. We assume that the envelope $f(z)$ is the same for the free and the bound Q2D electron (unchanged value of b_0) and the influence of the donor potential on the motion in the z direction is calculated in

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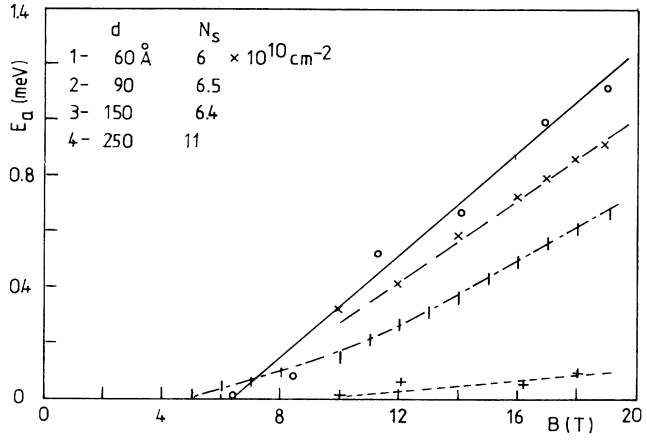

FIG. 1. Experimental activation energies of Si donors vs magnetic field for four GaAs-$Ga_{1-x}Al_xAs$ heterostructures with a spacer. The spacer widths d and the surface electron densities N_s at the metal-nonmetal transition are indicated. The lines are drawn to guide the eye.

the first-order perturbation theory. As shown by Brum *et al.*[9] this ansatz allows one to calculate the donor binding energy without knowledge of the confining potential in inversion layer. For b_0 we use the Stern-Howard expression $b_0^3=48\pi m^* e^2(N_d+0.34N_s)/\kappa_0 h^2$, where N_d is the depletion charge density.[10]

The static screening of the Coulomb potential is described using the procedure of Price[11] (the effect of magnetic field on the screening is not taken into account). After some manipulation one obtains the potential averaged over z in the form (in units of Ry*)

$$\tilde{V}(\rho)=-\int_0^\infty \left[1+\frac{q}{b_0}\right]^{-3}\frac{J_0(q\rho)\exp(-qd)dq}{1+P(q)H(q)}\ , \tag{1}$$

where J_0 is the Bessel function. The factor $(1+q/b_0)^{-3}$ comes from averaging over $f^2(z)$. The function $H(q)=(1+8q/3b_0)^{-1}$ represents "the screening of the screening" and it is related to the electron motion in the z direction. Finally, $\Pi(q)$ is the polarization function. In the freeze-out regime the Fermi energy is below the lowest Landau level, so that one deals with the nondegenerate electron statistics. For this case we calculate

$$\Pi(q)=-\frac{N_s}{kT}\Phi\left[1,\tfrac{3}{2},-\frac{\hbar^2q^2}{8m^*kT}\right]\ , \tag{2}$$

where Φ is the degenerate hypergeometric function. The binding energy is (in units of Ry*)

$$E_b=\gamma-T(\alpha,\beta)-U(\alpha,\beta)\ , \tag{3}$$

where R and U are trial averages of kinetic and potential energies, respectively. For GaAs electrons in the ground electric subband we take $m^*=0.07m_0$, $\kappa_0=12.56$, 1 Ry* = 5.8 meV.

In Fig. 3 we plot calculated binding energies of magneto-donors for GaAs-$Ga_{1-x}Al_xAs$ heterostructure with a spacer $d=150$ Å, a fixed typical depletion density $N_d=6\times10^{10}$ cm^{-2}, the temperature $T=4.2$ K, and different surface densities N_s. It can be seen that at lower N_s the theoretical binding energy depends very strongly on surface density and, in order to reach an even rough agreement with the observed values (sample 3 in Fig. 1), the inclusion of screening is essential. The above mentioned saturation of E_b at higher fields is seen.

In Fig. 4 we show the calculated binding energies of magneto-donors for four different spacer widths corre-

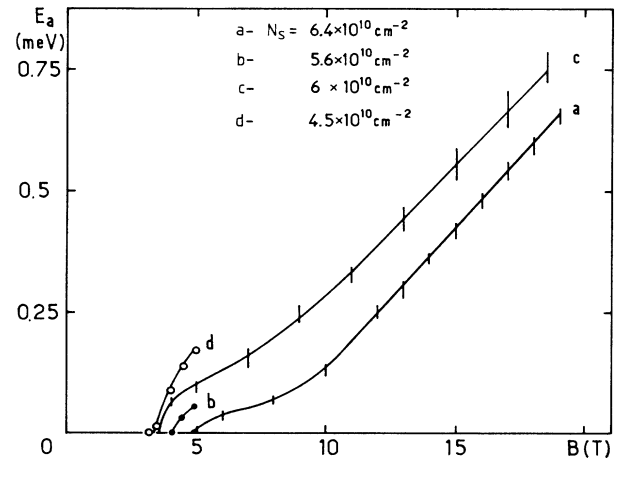

FIG. 2. Experimental activation energies for sample 3 (under pressure of 8.8 kbar) vs magnetic field. Different $E_a(B)$ dependences correspond to various N_s values at the metal-nonmetal transition achieved by different speeds of cooling of the sample. The lines are drawn to guide the eye.

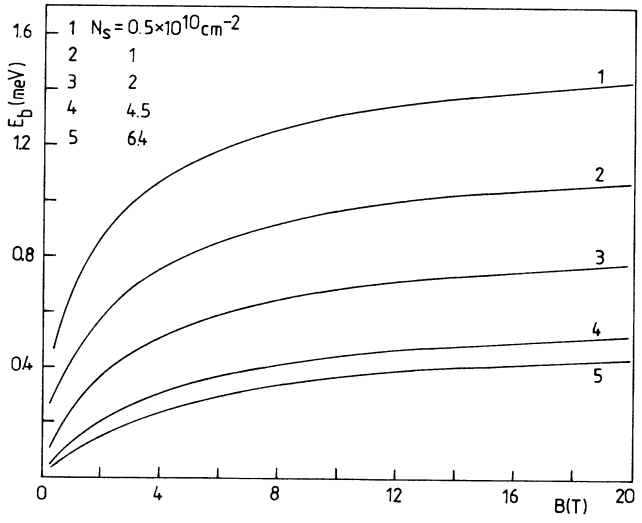

FIG. 3. Theoretical binding energies of magneto donors in a GaAs-$Ga_{1-x}Al_xAs$ heterostructure with a spacer $d=150$ Å and $N_d=6\times10^{10}$ cm^{-2} vs magnetic field, calculated for different surface densities N_s including screening.

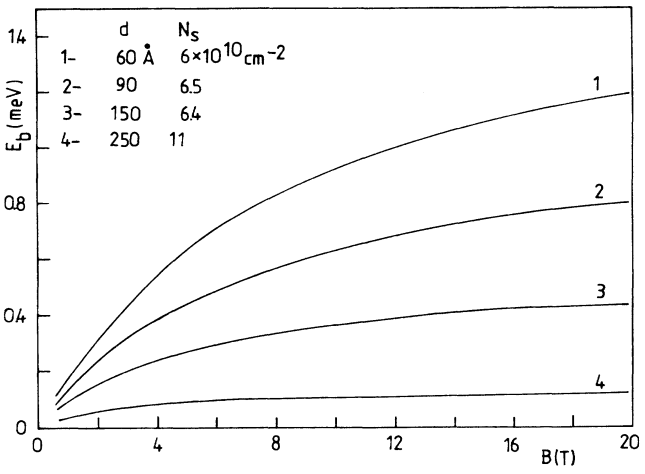

FIG. 4. Theoretical binding energies of magneto donors in GaAs-$Ga_{1-x}Al_xAs$ heterostructures vs magnetic field, calculated for spacers d and surface densities N_s indicated in Fig. 1 and $N_d = 6\times 10^{10}$ cm^{-2}.

sponding to d and N_s of the investigated heterostructures. Comparing these with the data in Fig. 1 one can see that at high fields, i.e., away from the metal-nonmetal transition, the theory describes quite well the experimental values. For example, at the field of $B \approx 16$ T the ratio of E_b for samples 1 and 4 is about 10, which is almost exactly reproduced by the theory. In view of the uncertainty concerning the real positions of Si donors responsible for the electron binding and the validity of the one-donor–one-electron picture even at higher fields, the agreement should be considered as surprisingly good. For higher spacers the saturation values are reached at lower fields, which is well confirmed by the experimental flat $E_b(B)$ dependence for sample 4.

The above theory underestimates somewhat the binding energies at high fields. In reality, as mentioned above, the electron is pushed toward the donor by the joined influence of magnetic field and the Coulomb interaction, which increases E_b. The interface GaAs-$Ga_{1-x}Al_xAs$ prevents this to a great extent but, keeping the same value of the parameter b_0 for the free and bound states, we ignore this effect entirely.

It is clear that, as B decreases, the one-donor–one-electron picture breaks down: the magneto-donor wave functions become bigger, their overlap increases, the ground state is broadened, the binding energy decreases and, finally, the nonmetal-metal transition occurs. This explains why at lower fields the experimental energies are smaller and the $E_b(B)$ dependences are steeper than the theoretical ones.

As follows from Fig. 3 the dependence of E_b on N_s becomes weak in the range of $N_s \approx 5\times 10^{10}$ cm^{-2}. This is due to the fact that with increasing N_s the value of b_0 in the wave function $f(z)$ increases, the electron is on average closer to the interface (i.e., also to the donor), which partly counteracts the effect of stronger screening. At high N_s the two factors almost cancel each other. Thus we believe that the dependence of E_b and N_s shown in Fig. 3, more pronounced than the one predicted theoretically for this range of electron densities, is related to the overlap of the wave functions. This effect is quite well known from the bulk studies of magneto-donors at higher densities (cf., e.g., Robert *et al.* [12]).

The fact that the measured donor activation energies depend only on B and on the initial free-electron density N_s, although in a freeze-out experiment N_s decreases more than an order of magnitude, seems to contradict our screening theory. However, the screening properties are determined by a polarizability of the system which is, in turn, proportional to its volume. In our case the volume is almost the same for free and bound electron states, since it is in both cases mainly determined by magnetic field ($a_\perp \simeq L$) and the inversion potential. Thus the screening is insensitive to the fact that the electrons are frozen-out from the Landau states to the bound states. The insensitivity of E_b to T at low temperatures results explicitly from the theory. Our treatment of screening goes further than that used by Kremer and Wallis,[13] but in a complete theory influence of magnetic field on the polarizability should clearly be included.

We have neglected an exponentially small penetration of the electron wave function into the barrier region. This simplification is not significant as the barrier height is few hundreds of meV, while we deal with the binding energies of 1 meV.

It is known from bulk investigations that optical donor energies are usually higher than those determined by transport measurements. We have calculated also energies of excited magneto-donor states, but optical data on GaAs-$Ga_{1-x}Al_xAs$ structures with a spacer are not yet available to our knowledge.

Our findings can be summarized in the following way: inclusion of screening of the Coulomb interaction between Si ions and inversion electrons is absolutely necessary for the description of the observed binding energies of magneto donors. At the experimentally achievable surface densities of $N_s = 5\times 10^{10}$ cm^{-2} or higher, the overlap of the magneto-donor wave functions is also of importance, leading to the nonmetal-metal transition at lower magnetic fields. Our results provide the direct evidence for the static screening of Coulomb interaction in Q2D systems, the electron mobility studies of inversion layers being always obscured by uncontrolled scattering modes, like surface roughness, defects, phonons, etc. In the investigated Q2D geometry the screening of the donor potential is particularly effective since the spacer keeps the electrons away from the ions.

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[1]N. C. Jarosik, B. D. McCombe, B. V. Shanabrook, J. Comas, J. Ralston, and G. Wicks, Phys. Rev. Lett. **54**, 1283 (1985).

[2]B. D. McCombe, N. C. Jarosik, and J. M. Mercy, in *Two-dimensional Systems: Physics and New Devices,* edited by G. Bauer *et al.* (Springer-Verlag, New York, 1986), p. 156.

[3]R. L. Greene and K. K. Bajaj, Phys. Rev. B **31**, 913 (1985).

[4]W. Rösner, G. Wunner, H. Herold, and H. Ruder, J. Phys. B **17**, 29 (1984).

[5]J. L. Robert, A. Raymond, L. Konczewicz, C. Bousquet, W. Zawadzki, F. Alexandre, I. M. Masson, J. P. Andre, and P. M. Frijlink, Phys. Rev. B **33**, 5935 (1986).

[6]J. M. Mercy, C. Bousquet, J. L. Robert, A. Raymond, G. Gregoris, J. Beerens, J. C. Portal, P. M. Frijlink, P. Delescluse, J. Chevrier, and N. T. Linh, Surf. Sci. **142**, 298 (1984).

[7]R. Mansfield, J. Phys. C **4**, 2084 (1971).

[8]Y. Yafet, R. W. Keyes, and E. N. Adams, J. Phys. Chem. Solids **1**, 137 (1956).

[9]J. A. Brum, G. Bastard, and L. Guillemot, Phys. Rev. B **30**, 905 (1984).

[10]F. Stern and W. E. Howard, Phys. Rev. **163**, 816 (1967).

[11]P. J. Price, J. Vac. Sci. Technol. **19**, 599 (1981).

[12]J. L. Robert, A. Raymond, R. L. Aulombard, and C. Bousquet, Philos. Mag. B **142**, 1003 (1980).

[13]G. M. Kremer and R. F. Wallis, Phys. Rev. B **32**, 3772 (1985).