Coulomb interaction and electronic phase transitions in quantum-well systems

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The effect of the Coulomb interaction of electrons on the positions of energy levels and on the localization of the wave function in systems of several quantum wells is studied. If the distance between the extrema of two lower subbands of the energy spectrum is smaller than a critical value characterizing the strength of the interaction, a Coulomb instability occurs in the system and leads to an electronic phase transition.

1. The outlook for the development of fundamentally new semiconductor devices based on heterostructures containing several quantum wells depends on reaching an understanding of the physical processes which occur in such systems. In most cases, an adequate description can be found[1,2] by the envelope method for the wave function, in which the layered heterostructure is modeled by specifying the potential energy for electrons in the form of a 1D single-particle potential. That method has the advantage over (for example) calculations by the strong-coupling method that the original properties of the semiconducting materials are taken into account correctly through empirical parameters such as the width of the band gap. Finding satisfactory results in calculations of the energy spectrum and wave functions requires consideration of the Coulomb interaction of the charge carriers. Since all the effects described below can be found even in the Hartree approximation, we will ignore the exchange interaction, which causes no qualitative changes in the picture.

2. The wave function of an electron in a system of quantum wells in the envelope method is written

$$\Psi(x, \mathbf{r}) = S^{-1/2} \sum_j \psi_j(x) \exp(i\mathbf{k} \cdot \mathbf{r}), \tag{1}$$

where S is a normalized area, and j is the index of the transverse-motion subband (transverse with respect to the axis of the quantum well), characterized by a quasimomentum $\mathbf{k}$. We are ignoring the spin of the electrons. The x axis runs along the axis of the structure, and we have $\mathbf{r} = (y, z)$.

The longitudinal component $\psi_j(x)$ of wave function (1) satisfies the equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_j(x) - \left[\epsilon - \frac{\hbar^2\mathbf{k}^2}{2m} - U_0(x) + e\phi(x)\right]\psi_j(x) = 0, \tag{2}$$

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where m and e are the effective mass and charge of an electron, and $U_0(x)$ is the original potential of the heterostructure. The electrostatic potential $\phi(x)$ is found from the equation

$$\frac{d^2}{dx^2}\phi(x)=\frac{4\pi e}{\kappa}[n(x)-N^+(x)], \tag{3}$$

where κ is the permittivity, and $N^+(x)$ is the concentration of ionized donors. For simplicity we consider the case in which the temperature T, expressed in energy units, lies in the interval $E_{\text{imp}} \ll T \ll \delta$ (E_{imp} is the ionization potential of an impurity atom, and δ is the distance between extrema of the two low-lying electron subbands). This condition holds over a broad temperature range up to room temperature for impurities such as Si in GaAs for quantum-well widths less than 10 nm. In this case all the donors are ionized, and their concentration is equal to the concentration of the dopant: $N^+(x)=N(x)$. In addition, all the electrons are in the lower subband of the energy spectrum, and the electron density $n(x)$ is given by

$$n(x)=\frac{2}{(2\pi\hbar)^2}\int f_j(\mathbf{k})d^2\mathbf{k}\,|\psi_j(x)|^2, \tag{4}$$

where $f_j(\mathbf{k})$ is the electron distribution function in subband j of the quantum-well system.

We expand the unknown wave functions $\psi_j(x)$ in the set of functions $\psi_j^{(0)}(x)$, which satisfy the equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_j^{(0)}(x)-[\epsilon_j^{(0)}-U_0(x)]\psi_j^{(0)}(x)=0. \tag{5}$$

In the expansion we retain only the two low-lying states $\psi_1^{(0)}(x)$ and $\psi_2^{(0)}(x)$, which play a leading role in shaping the states with broken symmetry. This approach is legitimate if the distance to the other subbands of the energy spectrum is greater than δ ; this condition can always be satisfied through a suitable choice of the parameters of the quantum wells. We can then write

$$\psi_1(x)=u\psi_1^{(0)}(x)+v\psi_2^{(0)}(x), \tag{6}$$

$$\psi_2(x)=u\psi_2^{(0)}(x)-v\psi_1^{(0)}(x), \tag{7}$$

$$u^2+v^2=1. \tag{8}$$

As a result, we find a system of equations for determining the coefficients u and v:

$$\left(\epsilon-\epsilon_1^{(0)}-\frac{\hbar^2\mathbf{k}^2}{2m}-\sigma_1\right)u-\gamma v=0, \tag{9}$$

$$\left(\epsilon-\epsilon_2^{(0)}-\frac{\hbar^2\mathbf{k}^2}{2m}-\sigma_2\right)v-\gamma u=0, \tag{10}$$

where

$$\sigma_i = \int_{-\infty}^{\infty} [\psi_i^{(0)}(x)]^* e\phi(x)\psi_i^{(0)}(x)dx, \tag{11}$$

$$\gamma_{ij} = \int_{-\infty}^{\infty} [\psi_i^{(0)}(x)]^* e\phi(x)\psi_j^{(0)}(x)dx = \gamma_{ji} \equiv \gamma. \tag{12}$$

As an example we consider a system of two identical quantum wells, and we demonstrate certain properties of the resulting solutions. We consider the typical case in which the quantum wells are uniformly doped by a donor impurity; i.e., we have $N(x) = N_0$ inside a quantum well and $N(x) = 0$ outside it. To study the conditions for the onset of states with a broken symmetry (with respect to mirror reflection) in the system, we replace the charge distribution in each quantum well and in the separation barrier by constant values, equal to the corresponding average values, and we ignore the charge in the outer barriers. A direct integration of Eq. (3) then yields the distribution of the electrostatic potential in this system:

$$\phi(x) = uv\phi_0(x), \tag{13}$$

$$\phi_0(x) = \begin{cases} \pm 2\pi N_0(e/k)[(x-a/2-d)^2 - (a+d)d/2], & x \in A, B, \\ 2\pi N_0(e/k)xd, & x \in C, \end{cases} \tag{14}$$

where A, B, and C represent respectively the quantum wells (a is the width of one well) and the region of the separation barrier (d is the barrier thickness). Since the potential in (14) changes sign upon mirror reflection in the $x = 0$ plane, which passes through the middle of the central barrier, the off-diagonal matrix elements γ in Eqs. (9) and (10) are nonzero. According to (13), they are proportional to uv. System of equations (9) and (10) then has nontrivial solutions for the parameter v under the conditions

$$\epsilon = \epsilon_0 + (\sigma_1 + \sigma_2 \pm \gamma_0)/2, \tag{15}$$

$$\gamma_0 > \delta + \sigma_1 - \sigma_2, \tag{16}$$

where

$$\gamma_0 = \int_{-\infty}^{\infty} [\psi_1^{(0)}(x)]^* e\phi_0(x)\psi_2^{(0)}(x)dx, \tag{17}$$

and where we have expressed the eigenvalues $\epsilon_{1,2}^{(0)}$ for the problem with a two-well potential in terms of the original distance between levels, δ (this distance depends on only the parameters of the separation barrier[3]) and in terms of the energy of a level in an individual well, ϵ_0:

$$\epsilon_{1,2}^{(0)} = \epsilon_0 \pm \delta/2. \tag{18}$$

If the distance between extrema of the electron subbands, δ, as renormalized by the diagonal Coulomb interaction, is smaller than the nondiagonal interaction, characterized by the parameter γ_0, then there are two types of solutions for the ground-state wave function: one which preserves the original symmetry of the structure and one

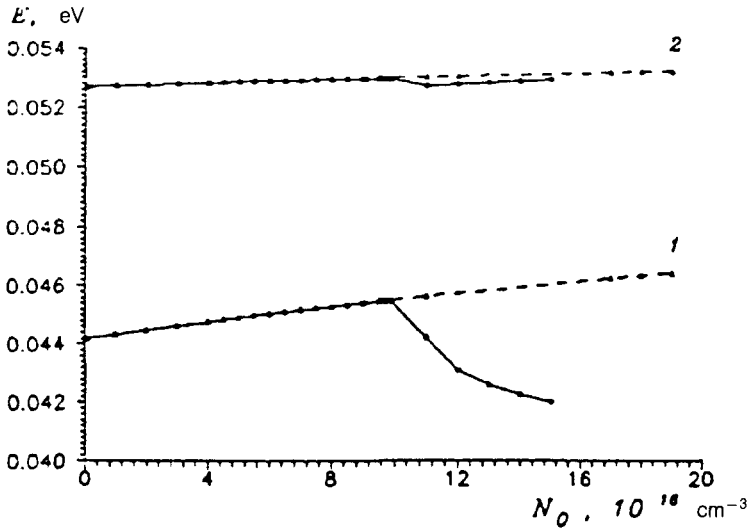

FIG. 1. Energy of the bottom of the subband as a function of the doping level N_0 for the first two subbands of the energy spectrum of a three-well test structure at $T=10$ K. 1—ϵ_1; 2—ϵ_2. The dashed lines are the corresponding curves for an unstable symmetric "parent phase" near the point of the phase transition.

which does not (we will refer to these solutions as respectively "symmetric" and "asymmetric"). Comparing (15) with seed spectrum (18), we see that under the condition

$$\gamma_0 > \delta + \sigma_1 + \sigma_2 \tag{19}$$

the asymmetric state is preferred from the energy standpoint. In other words, the system is unstable with respect to symmetry breaking. Since the structure has macroscopic dimensions in the plane of the quantum wells, and since a macroscopic number of electrons participate in forming the asymmetric state, this circumstance can be regarded as the existence of an electronic phase transition of a Coulomb nature in the system.

3. The conclusions reached on the basis of the analytic calculation can be extended to systems with a large number of quantum wells, as is confirmed by the results of a numerical simulation. The Schrödinger and Poisson equations for a system of quantum wells were solved by an iterative procedure. We studied the positions of the discrete energy levels, the shape and features of the localization of the wave functions, and the distribution of the electron density and of the self-consistent Coulomb potential as a function of the temperature, the doping level, and the dopant distribution. We simulated systems with two, three, and more quantum wells. We studied the cases of a uniform doping of the entire heterostructure, of doped barriers, and of doped quantum wells. We studied temperatures from absolute zero up to well above room temperature. In all cases we observed a qualitative agreement between the analytic and numerical results. As an example to demonstrate the changes which occur in the

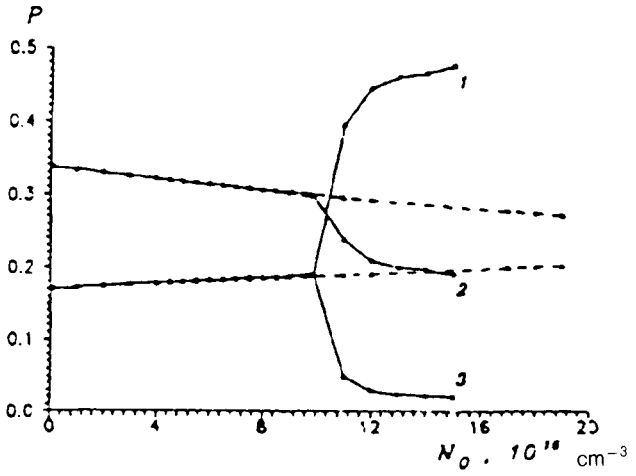

FIG. 2. Relative probability P for the filling of quantum wells as a function of the doping level N_0 for a 3D test structure. *1,3*—Side wells; *2*—central well. $T=10$ K. Dashed lines—Corresponding curves for an unstable symmetric "parent phase" near the point of the phase transition.

system in the course of the electronic phase transition, we consider a structure of three uniformly quantum wells which are symmetric under reflection in the plane perpendicular to the axis of the wells. The width of the wells and the width of the barriers between them are 5 nm, and the height of the barriers is 0.1 eV.

Anomalies which we regard as indications of an electronic phase transition arise along the scales of both the temperature and the doping level. At a low doping level (at a sufficiently high temperature) there exists a unique solution for the wave functions and the self-consistent potential. The symmetry of these wave functions is that of the original structure. With increasing dopant concentration (with decreasing temperature), we see a tendency for the energies of the two lower states to approach each other and for the probabilities for the filling of the quantum wells to become equal. Figures 1 and 2 demonstrate the behavior of the energies of the extrema of the first two subbands (the energy is reckoned from the bottom of the quantum well) and of the probabilities P for the filling of the quantum wells as a function of the doping level N_0 for a test structure at $T=10$ K. For a dopant concentration above the critical level, $N_0>N_c$ (in the case at hand, $N_c=10^{17}$ cm^{-3}), we find, in addition to the symmetric solution (the dashed line), two energy-degenerate solutions which do not preserve the symmetry of the system but which are mirror reflections of each other. Similar effects are found as the temperature is varied. Figure 3 shows a phase diagram for the test structure in the doping-temperature plane.

An important indication of the onset of a Coulomb instability is a change in the nature of the iterative process of the numerical solution of the system of Schrödinger and Poisson equations. At the point of the phase transition, the iterative process loses its convergence, becoming oscillatory. That these oscillations are physical in nature

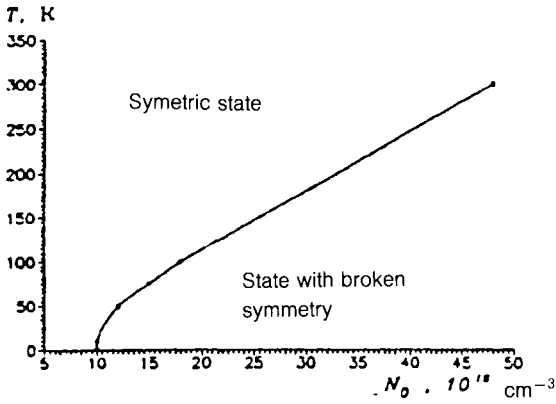

FIG. 3. "Phase diagram" for a test structure consisting of three quantum wells in the temperature-doping plane.

can be seen by solving Eqs. (9) and (10) by perturbation theory. With increasing order of the iteration, n, the coefficients v behave in the following way:

$$v^{(n+1)} = -v^{(n)}\gamma_0/(\delta+\sigma_1+\sigma_2). \tag{20}$$

In other words, the terms of the perturbation-theory series grow, changing sign in each successive iteration. Obtaining stable solutions requires a correct consideration of the off-diagonal terms in (9) and (10).

The physical reason for the instability and the further restructuring of the wave functions and the energy spectrum of the system is the Coulomb attraction of isolated donors in the side quantum wells and of electrons filling the lower subband. These electrons are therefore distributed nearly equally among the three quantum wells for this structure. The electron density for the next subband is localized primarily in the side wells, so the advantage in terms of energy from the excitation of an electron from the lower subband may be offset by the energy of the Coulomb attraction of positive and negative charges.

When we introduce an electron spin in the calculation, we also find some additional magnetic solutions. Since these solutions are close in energy to the asymmetric spin-free states discussed above, however, whether a magnetic order can occur in the system of quantum wells can be resolved only by taking the exchange interaction into account.

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[1] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Halsted, New York, 1988).
[2] A. A. Gorbatsevich, V. V. Kapaev, and Yu. V. Kopaev, JETP Lett. **57**, 580 (1993).
[3] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Nauka, Moscow, 1989).

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