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# On the problem of the spontaneous exchange-driven electron interwell re-population in semiconductor quantum wells

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**Abstract.** We reconsider the problem of the so-called exchange instability in symmetric semiconductor quantum wells, that is, an earlier proposed mechanism of a spontaneous interwell electron re-population due to different carrier density dependence of the Hartree and exchange energies. We show that the instability presents only in straightforward Hartree–Fock calculations and disappears as one takes into account interwell electron correlations.

## 1. Introduction

The study of phase transitions in many-particle systems with Coulomb interaction has a long history. One can mention the spontaneous spin polarization transition in a low-density free electron gas proposed by Bloch [1], the Wigner crystallization in a one-component electron gas [2], the Peierls metal–insulator transition in a crystal [3], the Kosterlitz–Thouless transition in a two-component plasmas [4], the transition to an exciton dielectric phase in a semiconductor having similar electron and hole Fermi surfaces predicted by Keldysh and Kopayev [5] etc. All these works treated an ordinary bulk 3D situation. In the 1980s, when systems with reduced dimension attracted attention, a new electron transition was suggested that could take place in a semiconductor quantum well system [6, 7]. Using the Hartree–Fock approximation for the treatment of electron–electron interaction, the authors of the articles [6, 7] argued that due to different carrier density dependence of the Hartree and exchange energies, an interwell electron redistribution might take place under conditions of low carrier density, leading to a spontaneous breaking of electro-neutrality in the system.

The arguments used in [6, 7] were quite simple. Let us consider a symmetrical double-well system with electrons populating only the lowest size-quantized levels, at zero temperature. In the Hartree–Fock approximation, the ground-state energy of electrons in the wells is equal to

$$E = K + E_{Hartree} - E_{exchange} \quad (1)$$

where  $K$  is the kinetic energy of the electrons. The three terms in the right-hand part have different  $n$  dependence,

$n$  being the 2D electron density in the well. The kinetic energy of a degenerate 2D electron gas is proportional to  $n^2$ . The Hartree energy is simply the Coulomb interaction energy under the approximation of uniform electron charge distribution, that is, the ordinary electrostatic energy of the system under consideration. If one uses the jelly model for the positive background then the Hartree energy equals zero in the electro-neutral state when electrons are equally distributed between the wells<sup>†</sup>. If the neutrality fails due to carrier redistribution between the wells, then

$$E_{Hartree} \sim (\Delta n)^2$$

where  $\Delta n$  is a difference between the electron densities in the wells, because  $E_{Hartree}$  is equal simply to the energy of a plane capacitor constituted by two wells.

The last term in equation (1), the exchange energy, is proportional to  $n^{3/2}$  for 2D degenerate electron gas [8, 9]. So at a sufficiently low  $n$  the negative exchange energy increases more rapidly with  $n$  than other, positive members of equation (1). This means that under such conditions the electrons must move to one well, thus ensuring maximum carrier density there. The corresponding loss in the kinetic and electrostatic energies is overwhelmed by the gain in the exchange energy, so the total energy (1) decreases. This transition is sometimes called the exchange instability.

This simple picture, however, brings about questions. The most fundamental one is the following. It is clear from

<sup>†</sup> One can consider this as a definition of zero energy. It means that  $E_{Hartree}$  includes not only the electron–electron interaction energy, but also the energy of the electron interaction with the background and the electrostatic energy of the background itself.

above that the proposed exchange instability is an entirely electron phenomenon that does not include any change in the symmetrical positive charge distribution. But electrons interact via repulsive forces. What is then the source of the effective attraction between the electrons, which makes them move from two wells into one, breaking electro-neutrality? Really, the exchange instability is equivalent to the presence of an attraction between two negatively charged electron planes in the wells, but there is no source of such attraction in the system. The only real attractive force, that between electrons and ions, acts just in the opposite direction, trying to maintain the electro-neutrality and to equalize the electron populations in the wells.

We will show below that the answer to this question is that the approximations made during the derivation of the expression (1) in [6, 7] were too crude, and if one treats the electron–electron interaction more accurately, the exchange instability disappears. The weak point of equation (1) is that it completely neglects interlayer electron correlation energy and treats electrons in two wells as two identical separate systems, which is incorrect. The interlayer correlations decrease the energy of the state with equal electron population in the wells, making this state stable.

Our results support the conclusion of [10] where the authors also argued against the exchange instability from the point of view of the Hartree–Fock approximation. Our approach, however, is more general as we do not use any approximation in treating the electron–electron interaction.

## 2. Calculations

Let us consider a quantum well system similar to one used in [6], that is, a symmetrical double quantum well system where electrons occupy only the lowest size-quantized levels in the wells (even when all particles move to a single well), at zero temperature. We neglect an overlap of electron wave functions in different wells because interwell tunneling plays no role in the proposed mechanism of the exchange instability. Then one can treat the electron degree of freedom that corresponds to the direction perpendicular to the layers in a site representation with a site index,  $i$ , that can take only two values, 1 and 2, because the system contains two wells. For example, a one-electron wave function of a particle localized, say, in the well number 1, in this representation has the form

$$\chi_{\sigma}(\rho, i) = \xi_{\sigma}(\rho) \Delta_{1i} \quad (2)$$

where  $\sigma = \uparrow, \downarrow$  is a spin quantum number,  $\rho$  is an in-plane 2D electron coordinate vector,  $\xi_{\sigma}$  is a 2D wave function in the plane of the well and  $\Delta_{ij}$  is the Kronecker delta. The wave function for an electron in the second well has a similar form.

The electron Hamiltonian of the system in this representation can be written as

$$\hat{H} = \sum_{k=1}^N \frac{\hat{p}_k^2}{2m} + U = \hat{K} + U \quad (3)$$

where  $N$  is the number of electrons in the system,  $\hat{p}_k$  is the 2D in-plane momentum of the  $k$ th electron,  $\hat{K}$  is the kinetic

energy,  $U$  is the electron–electron interaction energy

$$U = \frac{1}{2} \sum_{k=1}^N \sum_{n=1}^N \{u_{11}(\rho_k - \rho_n) \Delta_{i_k i_n} + u_{12}(\rho_k - \rho_n) [1 - \Delta_{i_k i_n}]\} \quad (4)$$

where  $i_k = 1, 2$  is the site index of the  $k$ th electron,  $\rho_k$  is its 2D coordinate vector and  $u_{11}$  and  $u_{12}$  are intra- and interwell two-particle electron–electron interaction energies. In the simplest case of infinitely thin wells

$$u_{11}(\rho) = \frac{e^2}{\epsilon_0 |\rho|} \quad u_{12}(\rho) = \frac{e^2}{\epsilon_0 \sqrt{\rho^2 + d^2}} \quad (5)$$

where  $d$  is an interwell distance (the barrier width) and  $\epsilon_0$  is the dielectric constant of a medium surrounding the wells. If the well width is finite, the simple expressions (5) are no longer valid, but in any case

$$u_{11}(\rho) > u_{12}(\rho) \quad (6)$$

and this is the only their property which is important for us.

We assume that members with  $k = n$  responsible for electron self-energy are omitted from the sum in the right-hand part of equation (4) and from similar sums below.

The electron interaction energy with the positive background of the symmetrical double-well system is symmetric in site index and hence it does not change on carrier redistribution between the wells, so it is omitted in equation (3) as well as other invariable terms such as the electrostatic energy of the background itself. As we are going only to compare energies of different electron states in the system and not to calculate the absolute values of these energies, we omit such constant terms from the Hamiltonian. In other words, the one-electron energy in equation (3) is measured from the level of size quantization. Taking the Hamiltonian in the form (3) we neglect the boundary effects at the edges of the layers, which is not important for bulk effects such as the exchange instability.

Now our goal is to prove that for any electron state with all electrons in one well one can build another state with electrons equally populating both wells, which is lower in energy. We will call the first state the single well state, and the second one the symmetrical state. Then we will be able to conclude that no single-well state can ever be the ground state of the system in question and hence the proposed exchange instability cannot take place in reality because it would lead just to the formation of a single-well ground state.

The single-well state wave function that corresponds to a state with all electrons in, say, well number 1, must have the form

$$\psi_{sw} = \phi(\rho_1 \dots \rho_N) \Delta_{1i_1} \dots \Delta_{1i_N} \quad (7)$$

where  $\phi$  is a normalized 2D (in-plane)  $N$ -electron wave function that satisfies the antisymmetry condition at an interchange of any two particles.  $\phi$  depends also on spin variables of all particles but they are not explicitly shown here because the Hamiltonian is spin independent and the spins are not directly involved in the calculations.

It is easy to show why any  $N$ -electron single-well state wave function in our system has this form. Really, one can expand the wave function in terms of the Slater

determinants which describe different states of a non-interacting electron system with all  $N$  particles in the first well. Consequently, all determinants must include the one-electron wave functions from the first well, every one of which is given by equation (2). So each term in every Slater determinant that enters the  $N$ -electron single-well wave function contains  $\Delta_{1i_1} \Delta_{1i_2} \dots \Delta_{1i_N}$  as a common multiplier, and thus one comes to the expression (7) for the wave function as a whole.

Let us consider another  $N$ -electron wave function

$$\psi_s = \frac{1}{2^{N/2}} \phi(\rho_1 \dots \rho_N) (\Delta_{1i_1} + \Delta_{2i_1}) \dots (\Delta_{1i_N} + \Delta_{2i_N}) \quad (8)$$

with the same  $\phi$  as in equation (7). The trial function (8) describes a symmetrical state with equal electron populations in both wells. Let us now compare mean energies in the states  $\psi_{sw}$  and  $\psi_s$ .

It is clear that

$$\langle \psi_{sw} | \hat{\mathcal{K}} | \psi_{sw} \rangle = \langle \psi_s | \hat{\mathcal{K}} | \psi_s \rangle \quad (9)$$

because the 2D kinetic energy operator  $\hat{\mathcal{K}}$  acts only on  $\phi$ . In contrast, the Coulomb interaction energies in these two states differ. Using equation (4) one obtains, on the one hand,

$$\begin{aligned} \langle \psi_{sw} | \mathcal{U} | \psi_{sw} \rangle &= \sum_{i_1=1}^2 \dots \sum_{i_N=1}^2 \int d\rho_1 \dots \\ &\dots d\rho_N \mathcal{U} |\phi(\rho_1 \dots \rho_N)|^2 \Delta_{1i_1} \dots \Delta_{1i_N} \\ &= \frac{1}{2} \sum_{k,n=1}^N \int d\rho_1 \dots d\rho_N u_{11}(\rho_k - \rho_n) |\phi(\rho_1 \dots \rho_N)|^2. \end{aligned} \quad (10)$$

We assume here and later on that the summation over spin variables is included in the integration over  $\rho_s$ .

On the other hand,

$$\begin{aligned} \langle \psi_s | \hat{\mathcal{U}} | \psi_s \rangle &= \frac{1}{2} \sum_{k,n=1}^N \frac{1}{2^N} \sum_{i_1 \dots i_N=1}^2 \int d\rho_1 \dots \\ &\dots d\rho_N |\phi(\rho_1 \dots \rho_N)|^2 (\Delta_{1i_1} + \Delta_{2i_1})^2 \dots \\ &\dots (\Delta_{1i_N} + \Delta_{2i_N})^2 [u_{11} \Delta_{ik_i n} + u_{12} (1 - \Delta_{ik_i n})] \\ &= \frac{1}{8} \sum_{k,n=1}^N \sum_{i_k, i_n=1}^2 \int d\rho_1 \dots d\rho_N |\phi(\rho_1 \dots \rho_N)|^2 \\ &\quad \times [u_{11} \Delta_{ik_i n} (\Delta_{1i_k} + \Delta_{2i_k}) (\Delta_{1i_n} + \Delta_{2i_n}) \\ &\quad + u_{12} (1 - \Delta_{ik_i n}) (\Delta_{1i_k} + \Delta_{2i_k}) (\Delta_{1i_n} + \Delta_{2i_n})] \\ &= \langle \psi_{sw} | \hat{\mathcal{U}} | \psi_{sw} \rangle - \frac{1}{4} \sum_{k,n=1}^N \int d\rho_1 \dots d\rho_N |\phi(\rho_1 \dots \rho_N)|^2 \\ &\quad \times [u_{11}(\rho_k - \rho_n) - u_{12}(\rho_k - \rho_n)]. \end{aligned} \quad (11)$$

Since for given  $\rho_k$  and  $\rho_n$  the intrawell interaction  $u_{11}$  is always greater than the interwell one  $u_{12}$  (see equations (5)–(6)), the integrating function in the second term of the final expression is positive and hence the integral is also positive. This means that the mean electron–electron interaction energy  $\langle \mathcal{U} \rangle$  is less when electrons are symmetrically distributed between the wells than when they are all concentrated in a single well. As the kinetic energies in both states coincide (see equation (9)), we come to the conclusion that the energy of the single-well state

is always greater than that of the corresponding symmetrical state with the same in-plane wave function.

If one takes a more general trial wave function

$$\begin{aligned} \psi &= \phi(\rho_1 \dots \rho_N) [\sqrt{\alpha} \Delta_{1i_1} + \sqrt{\beta} \Delta_{2i_1}] \dots \\ &\dots [\sqrt{\alpha} \Delta_{1i_N} + \sqrt{\beta} \Delta_{2i_N}] \\ \alpha + \beta &= 1 \end{aligned} \quad (12)$$

then it is easy to find that

$$\begin{aligned} \langle \psi | \mathcal{U} | \psi \rangle &= \frac{1}{4} \sum_{k,n=1}^N \int d\rho_1 \dots d\rho_N |\phi|^2 \\ &\quad \times [(\alpha^2 + \beta^2) u_{11}(\rho_k - \rho_n) + 2\alpha\beta u_{12}(\rho_k - \rho_n)]. \end{aligned} \quad (13)$$

The interaction energy (13) has a minimum at  $\alpha = \beta = 1/2$ , that is, just in the symmetrical state. The kinetic energy corresponding to the wave function (12) does not depend on  $\alpha$  and  $\beta$ , so the full energy also has a minimum in this state. The existence of the minimum is a direct consequence of the fact that  $u_{12} < u_{11}$ , which holds for any non-zero interwell distance.

### 3. Discussion

The results of the preceding section show that for any given state of our system with all electrons in one well there is another state with the symmetrical electron distribution over wells and a lower energy. Hence the single-well state cannot be the ground state of our system, which means that the exchange instability cannot take place in it.

So a question arises of what is wrong with the arguments of [6, 7] (see section 1) that lead to existence of the instability. Our opinion is that the source of the error is in the neglect of the interlayer correlation energy that decreases the full energy of the symmetrical state as compared with its straightforward Hartree–Fock estimate used in [6]. The energy of the symmetrical state of the system has been calculated there simply as twice the energy of a single well with  $N/2$  electrons. This method of calculation is acceptable if the interwell distance,  $d$ , is much greater than  $r_n$ , the mean interelectron distance in the well ( $r_n \sim 1/\sqrt{n}$ ). In this case the interlayer correlations are negligible because the electric field produced by the electrons in one well becomes almost uniform at the position of the other well. However, an elementary estimate of different terms in equation (1) shows that the exchange instability could take place only when the electron density  $n$  is so low that  $r_n \sim d$  or  $r_n > d$  or, which is the same, when two wells are so close to each other that the interwell barrier width is of the order of or less than the intercarrier distance in the wells. But at the interwell distance  $d \sim r_n$  the field of the electrons in one well is still non-uniform in the other well, so there is no reason to neglect the interwell correlations. If one still forgets about them and describes electrons in both wells by identical wave functions, then maxima and minima of the charge densities in the wells will be in identical positions in the planes of two wells. If we described this quantum mechanical picture in classical terms, we would say that the electrons in different wells are situated ‘just in front of each other’ across the barrier.

To further clarify things, let us consider this situation in a system with thin barrier  $d \ll r_n$  and in the limit of low

electron density. It is well known that at a sufficiently low density a one-component electron gas experiences the Wigner transition to a crystalline phase [2, 11] where the particles form a periodical lattice with one electron in each site. If we now consider for example the 2D carrier concentration in the wells to be so low that the Wigner crystallization takes place in each of them, then within the simple approach described above both 2D electron crystals in two layers would be situated in a position with their sites just in front of each other at a distance much less than the mean inter-electron distance in the plane ( $d \ll r_n$ ). So it becomes clear that when one intends to treat electrons in different wells as identical and independent systems, actually one unintentionally introduces rigid interlayer correlations and does it in a way that is unfavourable from the point of view of the electron–electron interaction energy. In this example one could significantly reduce this energy in two manners: first, putting all electrons in one well; the mean interelectron distance then increases because  $r_n \gg d$ ; and second, keeping the electrons in two wells but changing the electron arrangement so that the electrons in one well are situated in front of empty places in the other.

The first way obviously leads to the single-well state, and the result of the second method can be approximated by the symmetrical wave function built as was shown above. Really, if we could look at the electrons in the system along the growth direction, we would notice that the electron structures in the plane are similar in the symmetrical and single-well states because both structures must simply coincide when the barrier width tends to zero. As our symmetrical wave function is just based on the electron in-plane arrangement in the single-well state, it accounts for the main features of the actual electron ordering in the symmetrical state as long as the barrier is thin, that is, just in the area of our interest.

These two states where the electron–electron correlations are properly taken into account are considerably closer in energy to the ground state of our system than the state we started from, that with the electrons in two wells treated as independent. Of these two, the electro-neutrality is broken in the single-well state so there is an electrostatic energy loss in it as compared to the electro-neutral symmetrical state that corresponds therefore to the minimum energy of all three states.

If the electron density in the wells is now increased above the threshold of the Wigner crystallization, there will be no 2D crystalline long range order any more. However, short range correlations in the in-plane electron distribution will survive, and so the above picture of the interwell correlations still holds although it may not be so evident.

Up to now we have spoken only about the interaction energy. Let us consider the electron kinetic energy in all three states. Evidently, there is a kinetic energy increase in the second and third states as compared to the first one because the Fermi energy in the  $N$ -particle gas is greater than twice the Fermi energy in the  $N/2$  one. However, this effect is not important because at low electron density the main factor is the interaction energy, otherwise no Wigner crystallization could ever take place. Really, the kinetic energy of a particle in the 2D electron gas is proportional to  $n$  whereas its Coulomb energy to  $\sqrt{n}$ .

We remind the reader that during all the discussion above we bore in mind the case of low carrier density and thin barrier, which is important for the study of the exchange instability. For thick barriers, the role of the interwell correlations is negligible.

From this point of view the reason for the difference between the results obtained in [6, 7] and those of the present paper is clear. One has only to adapt the general picture described above to the approximate Hartree–Fock scheme used in [6, 7].

The use [6] of two identical  $N/2$ -electron Slater determinants in two wells as an  $N$ -electron wave function allows us to partially take into account only the intralayer electron correlations<sup>†</sup> and the corresponding intralayer exchange energy. However, the interlayer correlation energy, another negative contribution to the full energy of the system, is completely lost in this state.

Let us now turn to the state with all  $N$  electrons situated within a single layer. Here all correlations are the intrawell ones and so all them are taken into account (approximately, of course) even within the Hartree–Fock method. As a result, there is a definite gain in the electron–electron interaction energy as compared to the preceding state. There is also some energy loss due to breaking of the electro-neutrality in the system but it is proportional to the barrier thickness,  $d$ , and hence is small for thin barriers. In contrast, the correlation energy gain is  $d$  independent. So evidently the single-well state is more advantageous in the small  $d$  limit than the previous one. This is just the result obtained in [6, 7].

Finally, our trial symmetrical wave function (8) based on the single-well  $N$ -electron in-plane wave function combines advantages of both preceding variants. On the one hand, it accounts for both intra- and interwell correlations in a good approximation because the actual electron ordering in the two-well system with a thin barrier is quite similar to the ordering in the  $N$ -electron single-well state, as we tried to show above. Actually, the symmetrical function accounts for the correlations as well as the  $N$ -electron single-well function because both are based on one in-plane wave function. On the other hand, in the symmetrical state there is no loss in the electrostatic energy because the system keeps electro-neutrality. This function better approximates the true ground state wave function of our system than the other two functions considered above, and it corresponds to the lowest energy value among all three states.

So one can conclude that the arguments leading to the exchange instability are based on the use of a poor approximation for the wave function of the electro-neutral state, which does not account for the interlayer electron correlations. The use of the better approximation for the function immediately removes the instability.

<sup>†</sup> The approximate Hartree–Fock method does not take into account any correlations caused by the Coulomb electron–electron interaction. However, the method includes the quantum correlation effect known as the exchange hole formation (see, for example, [12]), which follows from the Pauli principle and hence exists even in the ideal gas of fermions, decreasing the probability of finding two particles close to each other. In a gas of interacting particles, these quantum correlations manifest themselves in the exchange energy, which is hence a kind of correlation energy corresponding to the quantum correlations.

#### 4. Conclusion

We considered here the old-standing problem of the so-called exchange instability in symmetric quantum well systems [6, 7]. We showed that if one accurately calculates the electron–electron interaction energy with proper account of the interwell correlations, there is no exchange instability. Its appearance in the simple Hartree–Fock approach is connected with the overestimation of the symmetrical state energy due to complete neglect of the interwell correlations. We did not use any approximation in our treatment of the electron–electron interaction in the system.

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