COMMENTS

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Comment on ''Exchange instabilities in semiconductor double-quantum-well systems''

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Semiconductor double-quantum-well systems in the low-density regime are prone to magnetic and charge-transfer instabilities. While recent calculations, using both a pseudospin approach and a local-spin-density approximation (LSDA) [Phys. Rev. B **55**, 4506 (1997)] seem to rule out the instability towards a monolayer configuration, the present contribution is devoted to refuting this conclusion in the LSDA. In this approximation, it is found that there is a charge-transfer instability for barrier widths that are neither too small nor too large. [S0163-1829(98)07732-7]

In a recent contribution, Zheng, Ortalano, and Das Sarma[1] have considered various exchange-driven electronic instabilities in semiconductor double-layer systems in the absence of any external magnetic field. One of the main conclusions of their work is that there is no exchange-driven bilayer to monolayer charge transfer instability in the double-layer systems. In this Comment, we want to point out that according to our calculations (which in principle use the same approach and similar system parameters as Ref. 1), there is a charge-transfer instability in double-layer systems. Typical parameters for this instability are two-dimensional densities of $10^{10}/\mathrm{cm}^2$ and barrier widths of 80 Å.

Before presenting our results, we give a few details about our (numerical) calculations. We have solved in a self-consistent way the (effective) one-dimensional Schrödinger and Poisson equations of the double-quantum-well system. Exchange and correlation effects are included by using the local density approximation[2] (LDA) for the exchange-correlation potential of the density functional theory.[3] For the study of the paramagnetic and fully spin-polarized (ferromagnetic) configurations we use a parametrization[4] of the exchange-correlation potential based in the variational Monte Carlo results of Ceperley and Alder.[5] For the treatment of arbitrarily spin-polarized phases, we employ the spin-density LDA (LSDA), with the interpolation proposed by von Barth and Hedin[6] for the exchange-correlation potential at intermediate polarizations.

We have considered four different phases in this low-density regime: a bilayer paramagnetic phase, a bilayer ferromagnetic phase, and the two monolayer paramagnetic and ferromagnetic counterparts. In order to avoid any ambiguity in the search for the stability of the four phases, we have calculated the total energy of each.[7] For a given set of parameters (density N_s and barrier width d_b) we have chosen the one with the lowest energy as the ground state. Besides, and for a complementary characterization, we have defined two order parameters,

$$P_{\pm}=\frac{1}{N_s}\int_0^{\infty} dz[\,\eta(z)\pm\eta(-z)\,], \tag{1}$$

where N_s is the total bidimensional electronic density, and $\eta(z)=\rho_{\uparrow}(z)-\rho_{\downarrow}(z)$ is the local-density magnetization, with $\rho_{\uparrow}(z)[\rho_{\downarrow}(z)]$ being the density fraction of up (down) spin-polarized electrons. $z=0$ corresponds to the midpoint of the

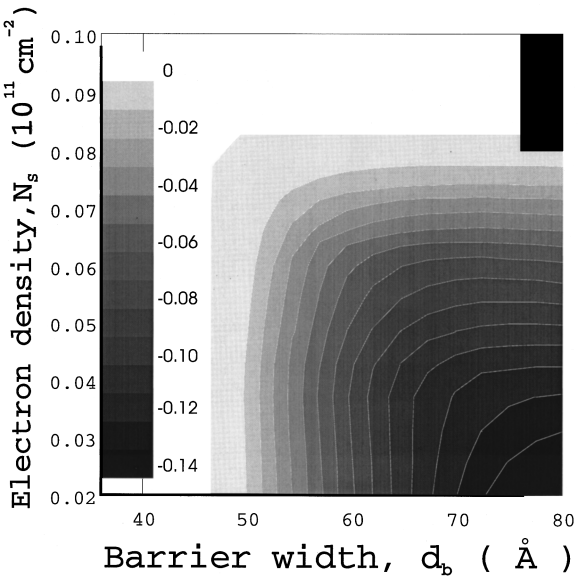

FIG. 1. Phase diagram (in parameter space) of the double quantum well, as a function of N_s and d_b. The shaded area covers the region where the monolayer ferromagnetic phase is the ground state, the gray intensity (in meV/particle) being proportional to the total-energy difference with the bilayer ferromagnetic phase. The rectangle in the upper right corner indicates the size of the grid. The remaining parameters are as follows: well width, $d_w=150$ Å; barrier high, 220 meV; coordinates of the delta-doped planes, $z=\pm(d_b/2+d_w+80$ Å).

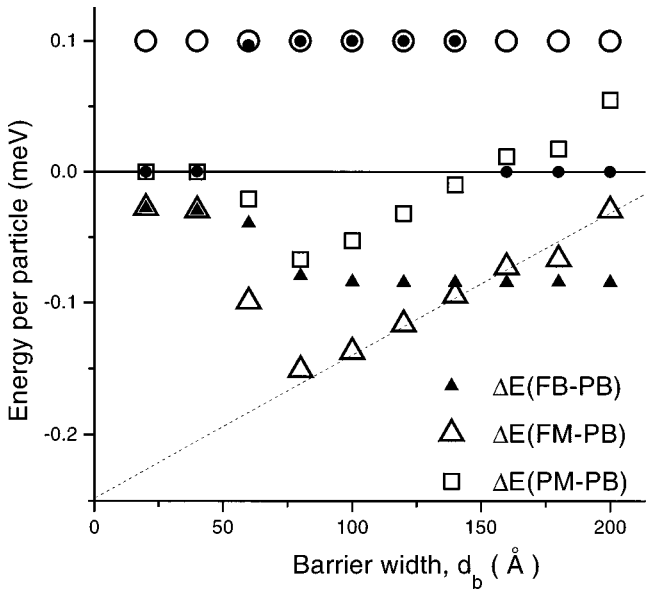

FIG. 2. Total-energy differences (per particle) with respect to the PB solution versus d_b for each one of the four possible configurations: PB: paramagnetic bilayer, PM: paramagnetic monolayer, FB: ferromagnetic bilayer, FA: ferromagnetic monolayer. The slope of the straight dashed line corresponds to Eq. (2) in the text.

barrier, which separates both two-dimensional electron gases. $P_+=P_-=0$ in both paramagnetic phases, while $|P_+|=1$ and $P_-=0$ in a fully polarized symmetric phase. Finally, $|P_+|=|P_-|=1$ in a fully polarized monolayer phase. In the case of partial polarization and/or not complete depopulation of a quantum well, $|P_+|$ and $|P_-|$ can take values close (but not equal) to unity.

Proceeding in this way, we have obtained the results shown in Figs. 1 and 2. Figure 1 compares the stability of both ferromagnetic phases, bilayer and monolayer, as a function of N_s and d_b. The intensity of the gray regions is proportional to the total energy difference per particle between both phases. According to these results, the bilayer ferromagnetic phase is unstable against the monolayer ferromagnetic phase for low enough densities ($N_s \lesssim 10^{10}/\mathrm{cm}^2$) and thick enough barriers ($d_b \gtrsim 50$ Å). None of the two paramagnetic phases is the ground state in the parameter space shown in Fig. 1. The bilayer paramagnetic configuration is stabilized at higher densities and smaller barrier widths; in this Comment we have concentrated our attention in the low-density regime of a double-quantum-well system, the intermediate-density regime ($10^{10}/\mathrm{cm}^2 \lesssim N_s \lesssim 10^{11}/\mathrm{cm}^2$) being treated separately.[8]

The results shown in Fig. 2 are complementary to those shown in Fig. 1. We display here the total energy of the four phases, referred to one of them (the paramagnetic bilayer phase), for a constant density ($N_s=0.06\times10^{11}/\mathrm{cm}^2$) and as a function of d_b. Note that in this case we have explored values of d_b larger than in Fig. 1; the order parameters defined by Eq. (1) are shown also.

The following features should be pointed out:

(i) For $d_b \lesssim 50$ Å, only bilayer phases are stable, with the ferromagnetic solution having a lower energy than the paramagnetic phase, and being therefore the ground state. The paramagnetic solutions were explored by starting from a perfect paramagnetic seed, as our self-consistent procedure preserves naturally this constraint. They are, however, unstable against small ferromagnetic perturbations: we have checked that if the seed has a small ferromagnetic component, the self-consistent procedure leads to an increase of the polarization, until convergence to a fully polarized ground state is attained. The degeneracy between the bilayer and monolayer phases (both for the paramagnetic and ferromagnetic cases), actually means that the self-consistent procedure always converges towards a bilayer solution (even when starting from an monolayer seed). Also note that $P_+=1$ and $P_-=0$, which is consistent with having a fully polarized bilayer ground state.

(ii) For 50 Å $\lesssim d_b \lesssim$ 150 Å, the ferromagnetic monolayer phase is the ground state of the double-quantum-well system, reaching optimum stability for some intermediate barrier width of about 75 Å. The paramagnetic monolayer phase has also a lower total energy than the bilayer solution, but this happens for a somewhat larger barrier width (as compared to the d_b where the ferromagnetic monolayer configuration becomes the ground state). For $d_b \gtrsim 75$ Å, it is important to remark that according to our calculations, both paramagnetic and ferromagnetic bilayer phases are metastable with respect to their respective broken symmetry counterparts. In other words, starting from a ferromagnetic seed with a small monolayer component, the self-consistent procedure converges towards the perfect bilayer solution, instead of falling towards the monolayer phase with lowest energy. The situation is analogous for both paramagnetic phases.

(iii) For $d_b \gtrsim 150$ Å, the bilayer ferromagnetic solution is again the ground state of the system. In contrast from the situation in the intermediate range of barrier widths, now both (para and ferro) broken symmetry solutions are metastable with respect to their respective symmetric (bilayer) counterparts.

As a summary of the results presented in Figs. 1 and 2, we see that the bilayer ferromagnetic phase is the ground state at small or large enough barrier widths, with the monolayer ferromagnetic phase being the ground state in the intermediate range of d_b. We discuss in what follows the physics behind such behavior and give some qualitative estimations to explain our results.

In the first place, it seems to be quite reasonable that the bilayer phases be the only solutions at small enough values of d_b: the electrons can tunnel easily through the barrier in this regime, so the kinetic energy cost associated with a monolayer solution is too large to be overcome by other effects. The stability of the bilayer phases for large enough d_b also looks quite reasonable, but for a completely different reason: in this regime, the larger energy corresponds to the classical Coulomb energy between the electronic charge distributions in both wells, which increases linearly with d_b in the monolayer situation. From simple electrostatic considerations we obtain for the difference between monolayer and bilayer phases the expression

$$\frac{\pi e^2 N_s}{2\varepsilon}(d_b+d_w), \tag{2}$$

which is positive and corresponds to the cost in energy associated with the charge transfer in going from a bilayer to a

monolayer configuration; ε is the dielectric constant of the well-acting semiconductor material (GaAs, $\varepsilon = 12.5$). To this we should add a negative d_b independent contribution, as the system gains exchange-correlation energy by going into the high-density asymmetric phases. The linear behavior with d_b is clearly seen in Fig. 2 for both the paramagnetic and ferromagnetic monolayer phases, for $d_b \gtrsim 100$ Å. The straight dashed line is just a plot of Eq. (2), where the negative exchange-correlation contribution has been adjusted to fit the calculated points. Two points should be clear with respect to this. First, we are adjusting the absolute vertical position of the dashed line and not its slope, which is obtained using Eq. (2). Second, the value we obtain for this negative exchange-correlation contribution is close to what can be estimated by assuming simple density distributions for the bilayer and monolayer configurations.

While we are quite confident about the results of our calculations, the source of the discrepancy with the conclusions of Ref. 1, where no instability towards monolayer phases were found is not clear to us. From our experience with this type of self-consistent calculations, we are, however, quite critical of the methodology used to explore the stability of the four phases. According to what is stated in Ref. 1, to search for the stability of the ferromagnetic phases, the self-consistency procedure was started from two seeds with different polarizations (10 % and 90 %). If both choices lead to a polarized final state, they conclude that the state is polarized. If only one choice leads to a polarized final state, they conclude that the result is not well defined, which gives rise to an uncertain region in their N_s versus d_b phase diagram equivalent to our Fig. 1. Nothing is said about how the stability of the monolayer phases is explored. This ''ad hoc'' procedure should be contrasted with our systematic methodology, where we calculated the total energy of each of the possible configurations, and chose the one with the lowest energy as the ground state of the system. Proceeding in this way, we never found a problem in assigning the character para/ferro bilayer/monolayer to any point in the N_s versus d_b phase diagram. Besides, it is important to note that for a broad range of parameters some phases are metastable with respect to the ground-state configuration. For instance, for $d_b \gtrsim 75$ Å, both paramagnetic and ferromagnetic bilayer phases are metastable against their respective monolayer counterparts. This means that unless one started from many quite different seeds and let the system attain full self-consistency, it is possible for the algorithm to become trapped in a local minima in configuration space.

The monolayer phase is a result of our rigorous application of LSDA theory to the double-quantum-well system; besides the clear conflict with similar calculations of Ref. 1, our results point out something that can be considered a more serious and deeper discrepancy. Zheng *et al.*[1] claim agreement (absence of the monolayer phase) between results obtained with two different methods: pseudospin description[9] for the layer degree of freedom (zero-tunneling approximation) in Secs. II and III, and LSDA formalism in Sec. IV. In light of our results, no such agreement exists between both treatments, and as the modelling of the system is much more realistic in the LSDA (for instance, tunneling is treated exactly), this casts some shadows on the accuracy of the pseudospin formalism as applied to the present problem.

In summary, within the framework of the LSDA, we have found that there is an exchange-correlation driven bilayer to monolayer charge transfer instability for the double-layer system in the low-density regime. As a function of barrier width, the instability appears in some intermediate range (50 Å $\lesssim d_b \lesssim 150$ Å). The results are at variance with recent claims presented in Ref. 1.

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