Localization of electrons and formation of two-dimensional Wigner spin lattices in a special cylindrical semiconductor stripe

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(Received 24 March 2010; revised manuscript received 9 June 2010; published 27 August 2010)

We consider a two-dimensional (2D)electron gas residing on the surface of a cylinder of a given radius R in the presence of a parabolic confinement along the axis of the cylinder. In this way the system of electrons forms a closed cylindrical stripe (wire). Using the local spin-density technique we first consider localization of electrons within of a potential barrier embedded in the wire. Barriers with sharp retangularlike features are populated in steps because of Coulomb blockade. The nature of a single bound state in a short soft barrier (quantum point contacts) at pinch-off is discussed in terms Coulomb blockade. For a shallow barrier-free wire we retrace the structural transitions at low electron densities from a single chain of localized states to double and triple chains (Wigner spin lattices). The present system is related to the model of a inhomogeneous quantum wire introduced recently by Güçlü *et al.* [Phys. Rev. B **80**, 201302(R) (2009)]. An important aspect is, however, the present extension into higher electron densities as well as to the low-density regime and the formation of 2D Wigner microlattices.

DOI: 10.1103/PhysRevB.82.073307 PACS number(s): 73.21.−b, 73.23.−b, 74.78.Na

The role of the many-body interactions in low-dimensional semiconductor nanodevices is well recognized (for recent overviews see[1,2]). For instance, delicate details of ballistic electron transport such as the 0.7 conduction anomaly in quantum point contacts (QPCs) may be understood only within the framework of many-body electron theory. The importance of spontaneous spin polarization was recognized already at the first observations of this phenomenon[3] and later this idea has been extensively developed by many authors.[1,2] Also here we will pursue this line.

Previous studies of the spin-polarization phenomena in QPCs, quantum wires, etc., have mostly focused on cases for which interaction-induced wave-function localization has been less prominent. In general these cases refer to strong geometric confinement and electron densities that are relatively high. More recently, however, the regime of *weak confinement* and *very low electron densities* has become accessible experimentally by the important development of high-mobility top gate heterostructures and QPCs.[1] Thus recent conductance measurements indicate the incipient formation of a Wigner electron lattice and row coupling in such systems.[4,5] Previously Wigner crystallization in low-dimensional structures has been anticipated on theoretical grounds. For example, the effect of exchange interactions on the conductance of a quantum wire in the Wigner-crystal regime has been studied by Matveev and collaborators.[6,7] Most recently Güçlü *et al.*[8] have performed quantum Monte Carlo simulation of an inhomogeneous quasi-one-dimensional (Q1D) single-mode system with the strong interactions and confinement. Q1D lattices with strong antiferromagnetic correlations appeared to be favored within a certain low-density barrier region (see below). Qualitatively, similar results have been obtained for the spin-Peierls transition in quantum wires and quantum rings by means of the self-consistent local spin-density approximation (LSDA).[9] (We recall that a spin symmetry-broken LSDA solutions reflect the true correlations inherent in the corresponding properly symmetry-restored state obtained from, for example, exact digonalization techniques. We will have this in mind as we discuss below, for example, antiferromagnetic states.[9]) In view of the experimental development there is an apparent need to extend previous studies to the regime of weak confinement and very low electron densities where interaction-induced localization of electrons is expected to be strong.

The outline of the presentation is the following. Below we describe the electron localization in a parabolic quantum wire with an embedded barrier[8] as well as the formation of a two-dimensional (2D) Wigner spin lattice in a barrier-free shallow wire. In both cases we have taken into account exchange-correlation potentials in accordance with LSDA (for details of a typical LSDA device modeling see, for example, Ref. 10). As a result, we have found interaction-induced multirow localization of electrons in the low-density regime. We have also followed the crossover between the localized and extended state regimes. As in Ref. 8 we have found the formation of a Q1D antiferromagnetic ordering (correlations) inside the barrier region and also shown that the localization is strongly dependent on the sharpness and length of the potential barrier. Localized states such as two distinct strands,[4,5] double zigzag and triple-row spin lattices have been demonstrated as well. There is a certain overlap of the first part of the present study with that of Güçlü *et al.*,[8] a circumstance that we utilize for validation and calibration of our approach. Because of the computational ease of LSDA we have readily extended previous simulations to higher electron densities. The second part of the Brief Report addresses the new regime of very low electrons densities and shallow confinement.

As a model, we consider a two-dimensional electron gas residing on the surface of a cylinder of a given radius R in the presence of a parabolic confinement along the y axis of the cylinder. In this way the system of electrons forms a closed cylindrical stripe. If a barrier region (gate potential) is introduced as in Ref. 8 we have the total confinement potential

$$V_{\text{conf}} = \frac{1}{2}m^*\omega^2 y^2 + V_g\{\tanh[s(\theta+\theta_0)] - \tanh[s(\theta-\theta_0)]\}, \tag{1}$$

where the first term is a transverse confining parabolic potential for electrons with effective mass m^* whereas the second term defines the barrier along the ring; s and V_g are parameters which specifies the steepness and the height of a barrier, θ is the azimuthal angle and θ_0 gives the position of the barrier. For later use we introduce the notation $x=R\theta$ with $-R\pi < x \leq R\pi$. Our model system is closely related to the choice of Güçlü *et al.*[8] In our case, however, we deal with a cylindrical geometry whereas they focus on a planar circular device. This difference may be of principle interest but as it turns out it has little impact on the final numerical results, in particular for large values of R. The model potential in Eq. (1) may generally be applied to a wide range of situations, from shallow 2D top gated devices[11,12] and wires to Q1D QPCs.[1] The above potential should be relevant also for the new generation of quantum rods and pillars that is forthcoming.

For later comparison with the results of Güçlü *et al.*[8] we choose parameters in the same range as used by them. Typically, the system has a circumference of 1.57 μm and is limited in the y direction to ± 40 nm. The barrier is effectively rectangular for s in the range of 4 or higher[8] but at lower values of s the edges become smoothed and eventually the barrier becomes more like a conventional QPC saddle potential.

In the present case spatial and spin distributions are obtained from the self-consistent solution of the Kohn-Sham (LSDA) equations for the occupied electron orbitals $\Psi_k^\sigma(\sigma = \pm\frac{1}{2})$,

$$H^\sigma \Psi_k^\sigma = E_k^\sigma \Psi_k^\sigma, \tag{2}$$

which obey cyclic boundary conditions. The single orbital Hamiltonian H^σ in Eq. (2) is the sum of the confinement potential [Eq. (1)], the usual kinetic-energy operator and the terms which describe the Coulomb, exchange and correlation energies in the 2DEG at a GaAS/AlGaAs interface (explicit forms for these terms may be found elsewhere, for example, in Ref. 10). The above self-consistent LSDA equations have been solved iteratively for a given chemical potential or number of electrons using numerical discretization. Convergence was ensured by repeated calculations for each set of parameters, each time starting with new separate random potentials for the two spin directions. It was found that the correlation potential is of great importance since ferromagnetic solutions were found without correlation whereas no such solutions could be found for the single chain when correlation was included. Furthermore, sufficient numerical resolution was achieved by increasing the number grid points until the same self-consistent results obtained.

In a first step we have analyzed the barrier population N as function of barrier height V_g at fixed values of the chemical potential μ. Integrating the total electron density $n(\mathbf{x})$ within the region $|\theta| < \theta_0$, one thus finds for steep barriers quite a distinct and rich steplike behavior of N as function of gate voltage V_g. The states within the barrier region are then well localized and disconnected from the outer region. The localization occurs already on a one-electron level because of the strong reflections and wave function buildup at the two ends of the barrier. Because of Coulomb blockade there is a step-wise filling of the states within the barrier as noted already in.[8] An extension to more electron rich cases are shown in Fig. 1 for three different values of the chemical potential. The degree of localization and number of electrons localized to barrier region obviously depend on the steepness parameter s and the height of the barrier V_g. For example, if s becomes smaller the separation between barrier and surrounding regions is blurred and there is a crossover to a smooth continuous filling of the barrier region, i.e., the barrier region becomes open (referred to as a "liquid state" by Güçlü *et al.*[8]). This also happens at higher fillings as indicated in Fig. 1 for $\mu=40$ meV. The special case of a remnant single bound state in the crossover region is discussed below.

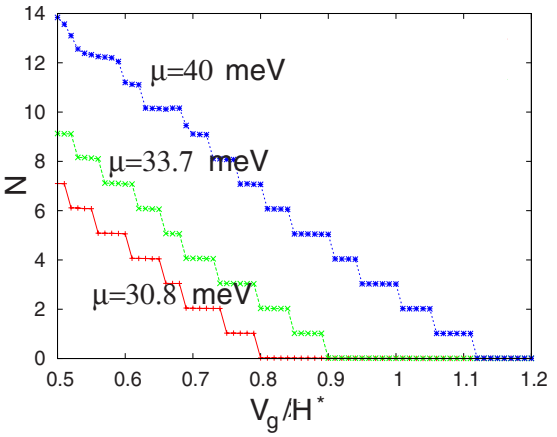

FIG. 1. (Color online) Number of electrons N inside a steep barrier with $s=15$ and $\theta_0=1.5$ as a function of a gate potential V_g in units of effective Hartree units H^* (=11.9 meV in GaAs).

We now turn to the question about spin and charge correlations among the electrons localized within the barrier, i.e., above pinch-off. We have searched for both antiferromagnetic and ferromagnetic order within a wide range of the parameters involved. Generally our LSDA results agree well with those of Güçlü *et al.*[8] which is as an important validation of our computational scheme. Thus we have found an abundance of charge-ordered antiferromagnetic LSDA solutions trapped by the two barriers. At the same time we were not able to recover ferromagnetic LSDA solutions for any of the parameters used. This result is in sharp contrast to similar LSDA simulations for conventional split-gate QPCs (Refs. 1 and 13) which seems to point to an important dependence on device geometry.

The pinch-off region is intriguing as discussed already in Ref. 8. Figure 2 shows an almost depleted barrier for $s=1.4$, i.e., a "soft barrier." At $s=2.4$, however, a single electron has entered the region, i.e., there is a distinct peak in the electron density corresponding to one electron residing inside the barrier. The corresponding wave function is to a good approximation a Gaussian function indicating a rather shallow parabolic potential in the interior of the barrier. In

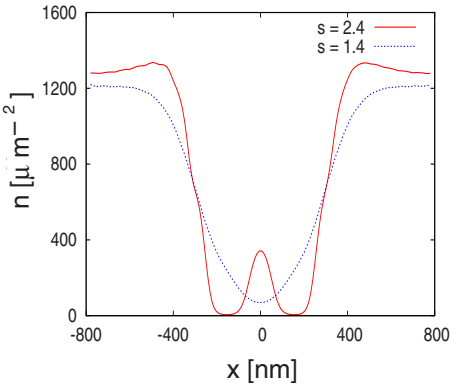

FIG. 2. (Color online) Density of electrons for $y=0$ for different steepness of the barrier ($s=1.4$ full curve; $s=2.4$ dotted curve; $\theta_0=1.3$) at fixed number of electrons (in both cases 15 spin-up and 15 spin-down electrons for $\mu=29.75$ meV); $\hbar\omega=7.14$ meV and $V_g=9.52$ meV.

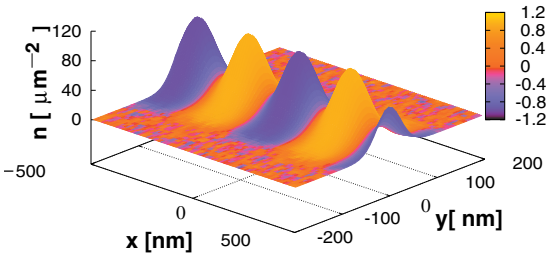

FIG. 3. (Color) Localization of four electrons (two up- and two down-spin electrons) in the wire without a barrier: $\hbar\omega=0.595$ meV.

addition, with increasing s the pile-up of charge and potential at the two ends of the barrier increase. As a consequence the localized state in Fig. 2 simply derives from electrostatic forces and Coulomb blockade. For this reason exchange and correlations potentials have little impact on this mechanism. Because of spin degeneracy an isolated state of this kind should therefore be a fluctuating one.

The single electron state in Fig. 2 is quite fragile. For example, we find that on increasing the electron density in the system for the given s value the peak quickly delocalizes. A slight softening of the potential has a similar effect. Figure 2 thus refers to a transition region in which localization is about to set in. Güçlü *et al.*[8] have suggested that the single peak is related to the Kondo scenario for the 0.7 conduction anomaly in QPCs.[14] Because of the unstable nature of the singly occupied localized state around pinch-off we rather propose that it is related to the conduction features discovered by Yoon *et al.*[15] at and below pinch-off of a QPC.

The cases above all refer to barriers embebbed in single-mode quantum wires with strong transverse confinement. We now turn to the case of shallow confinement that relates to certain 2D low-density top gate devices.[4,5,11,12] To accommodate more localized states we let $V_g=0$, a step that does not change the overall qualitative features. In the calculations we have assumed that the total number of electrons is fixed. Results for systems with $\hbar\omega=0.595$ meV containing 4, 16, and 44 electrons are shown in Figs. 3–5, respectively. The sequence shows how a single row of localized states in the four-electron system (two up- and two down-spin electrons in Fig. 3) transforms first to a double zigzag structure for 16 electrons (eight up-spin and eight down-spin electrons as in Fig. 4) and then to a more complex structures such as the triple-row microlattice for 44 electrons (22 up- and 22 down-spin electrons in Fig. 5). The wave functions corresponding to Figs. 3–5 are basically tight-binding states consisting of linear combinations of Gaussians functions, one for each electron and spin. The model may obviously be extended to large-size arrays of spins and realistic top gate 2D devices.[11,12]

The complex multichain structures in shallow wires occur because the electrons are given more space in which they may localize to reduce the interaction energy at little cost for the increase in kinetic and parabolic confinement energies. The very fact that "structural transitions" occur as the electron density is increased agrees in general terms with Monte Carlo simulations for classical screened particles[16] as well as for Heisenberg-type Hamiltonians.[6,7] The separation into, for example, spatially phase-shifted zigzag sublattices for up and down electrons as here is, however, a specific quantum feature in a regime that has not been explored previously within LSDA. The multichain structures should lead to unusual conductance crossovers as observed, for example, in Refs. 4 and 5 for shallow wires. This indicatse that there are more than one chain that contribute to total conductance. For specific cases with even number of electrons as, for example, in Fig. 4 we have found just antiferromagnetic arrangements of spins. For different number of electrons, odd or even, more complex charge and spin arrangements are found as discussed also in Refs. 6 and 7.

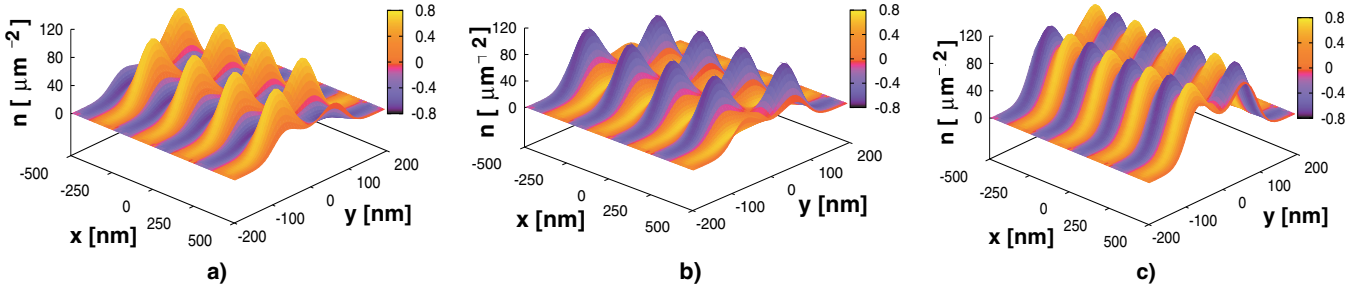

FIG. 4. (Color) Double zigzag structure in the case of a wire with 16 electrons (eight up- and eight down-spin electrons) for $\hbar\omega=0.595$ meV; (a) and (b) refer to up- and down-spin densities, respectively, and (c) to the total density.

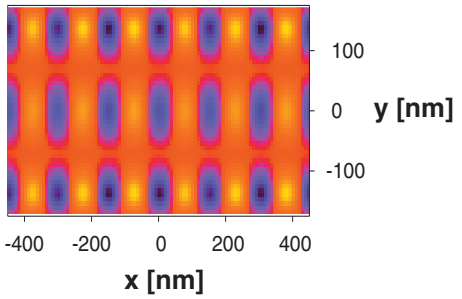

FIG. 5. (Color) Three row spin-lattice in the case of a wire with 44 electrons (22 up- and 22 down-spin electrons) for $\hbar\omega = 0.595$ meV.

In summary, the present results for the spatial electron distributions and spin correlations in a cylindrical wire with an embedded barrier are in a good qualitative agreement with the quantum Monte Carlo computations for an analogous circular ring[8] and for a finite Q1D ring with a small number of electrons.[9] Because of the ease of using LSDA we have been able to extend previous studies to a large number of electrons and different situations, from sharp barriers to shallow confinement at low densities. In the first case the localization within the barrier region is basically due to the strong reflections at the two ends of the barrier. These states are occupied by electrons one at a time and we have recovered an extended Coulomb staircase for this case. Spin correlations are generally antiferromagnetic in contrast to conventional split-gate QPCs.[1,2,10] This difference is an effect of the specific geometries used in the two cases. When the barrier in Eq. (1) is made softer the degree of localization decreases and eventually vanishes in the pinch-off region as in Fig. 2. In this region we also find a localized one-electron state as did Güçlü *et al.*[8] who associated this state with the Kondo scenario for the 0.7 conduction anomaly in a QPC.[14] We have found, however, that this state which derives from Coloumb blockade is very volatile and easily vanishes when, for example, the electron density is increased via V_g. For this reason we propose that the state might be related to the resonance observed by Yoon *et al.*[15] close to pinch-off and not to the Kondo mechanism as above.

In the case of cylindrical rings with shallow transverse confinement there is clear evidence of electron localization in the low electron-density regime where the Coulomb interaction energy overcomes the kinetic and parabolic confinement energies. On increasing the number of electrons there are structural transitions. Thus we have found interaction-induced bifurcations of single row (Fig. 3) into two (Fig. 4) and three (Fig. 5) distinct rows. Structures of these kinds may be responsible for the anomalous behavior in the shallow confinement limit for which conduction measurements suggest the formation of multichains[4,5] as well as impurity-assisted lattices.[11,12] These results invite further experimental and theoretical work, in particular, on ultralow density systems.

We are grateful for discussions with I. Abrikosov, H. U. Baranger, J. Bird, T. M. Chen, and M. Pepper and for support from the Swedish Research Council.

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