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Ground state properties of a laterally confined two-dimensional electron gas

L. Dandrea, F. Pederiva, and E. Lipparini
Dipartimento di Fisica and INFN, Università di Trento via Sommarive, 14, I-38100 Povo-Trento, Italy

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We present an accurate diffusion Monte Carlo computation of the ground state of a two-dimensional electron gas laterally confined by a harmonic potential in the effective mass-dielectric constant approximation. The computation is made explicitly including the second dimension, and can therefore address the occurrence of phase transitions in the system. The system was studied as a function of the one-dimensional Wigner-Seitz parameter $r_s = 1/2\rho^{1D}$ in the range $0.5 \leq r_s \leq 7$. The ground state is found to be spin polarized for $r_s > 3$.

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I. INTRODUCTION

The two-dimensional (2D) electron gas laterally confined by some potential is an important model in many-body physics, since the progress in nanostructure technology has allowed the fabrication of quasi-2D quantum stripes. Experiments performed on these nanostructures have pointed out the quantization of the conductance G in units of $2e^2/h$, which reflects the number of active channels in the transport measurements.[1–3] An anomalous conductance structure close to $G = 0.7(2e^2/h)$ has been observed in many cases.[4–9] This structure has given rise to many interpretations based on spontaneous spin polarization of the system mediated through the exchange-correlation interaction,[10–15] on possible manifestation of a Kondo effect,[16–18] or of Wigner crystallization of the confined electron gas at low density,[19] or of a Tomonaga-Luttinger liquid behavior.[20–29] All these results are based on specific models or approximations such as, for example, the local spin-density functional theory.

In this paper we address the problem by computing the ground state energy of a 2D-quantum stripe of infinite length and finite width by means of accurate fixed–node diffusion Monte Carlo (DMC) simulations. The stripe is described by a two-dimensional Hamiltonian of N interacting electrons laterally confined by a parabolic potential. The extension of the stripe in the third dimension is neglected, as in most theoretical descriptions. Within DMC, it is possible to calculate the ground state energy for the unpolarized and fully spin-polarized liquid and crystal phase. This enables us to determine, by comparing the energies, the density at which the electron gas in the stripe polarizes. Previous Monte Carlo calculations of quasiunidimensional systems have been performed by Casula *et al.*[30] The authors in that case considered a one-dimensional system with an interaction that effectively includes the width of the wire. However, the Hamiltonian being one-dimensional, no phase transitions can occur in the system, according to the Lieb-Mattis theorem.[31] Our calculation being fully two-dimensional, makes it possible to discuss relative stability of phases with different symmetry.

II. MODEL HAMILTONIAN

In order to determine the Hamiltonian of the system we start from a 2D electron gas of density $\rho^{2D} = 1/\pi a^2$ in the effective mass-dielectric constant approximations. In this paper we will consider effective units $\hbar = e^2/\epsilon = m_e m^* = 1$. The density of the gas is parametrized by the effective Wigner-Seitz radius in effective atomic units $r_s^{2D} = a/a_0^*$. For reasons of convenience, in the simulations we prefer to rescale all length in terms of a one-dimensional Wigner-Seitz parameter $r_s = L/2N$ where N is the number of electrons, and L is the length of the wire, which by this scaling depends only on the number of electrons, and not on the density. The one- and two-dimensional densities are related to each other as $\rho^{1D} = \rho^{2D} w(\rho^{1D})$, where w is an estimate of the width of the wire. A possible definition of $w(r_s)$ is given by twice the distance from the center of the wire at which the transverse density decays to one half of the value at the center. Similarly we can relate r_s^{2D} and r_s as $r_s^{2D} \sim \sqrt{2 r_s w(r_s)/\pi}$. With this choice of the length units, energies are given in effective Rydbergs. The Hamiltonian of the N electrons in the stripe is then defined as follows:

$$H = -\frac{1}{r_s^2}\sum_{i=1}^{N} \nabla_i^2 + \sum_{i=1}^{N} \hat{\omega}_0^2 y_i^2 + \frac{2}{r_s}\sum_{i<j}^{N} \frac{1}{|\mathbf{r_i} - \mathbf{r_j}|}. \quad (1)$$

The harmonic confinement parameter $\hat{\omega}_0 = \omega_0 r_s$ is scaled consistently with the coordinates. Note that for independent electrons this choice of the confinement would give a width of the wire $w(r_s) \propto 1/r_s$, therefore corresponding to maintaining constant the two-dimensional density. The infinite extension along the x direction is accounted for by using a modified version of the Ewald summation. The assumption is that the diverging Coulomb repulsion is compensated by the interaction with a jellium of positive charge. We then consider a 2D array of such stripes in the limit of infinite separation. Part of the resulting potential must be computed numerically at the beginning of the simulation.

III. COMPUTATIONAL METHODS

The computation follows the standard procedure for quantum Monte Carlo (QMC) calculations, using a modified version of CHAMP.[32] The first stage consists of minimizing the expectation of the Hamiltonian over a trial state of the following form:

$$\psi_T(\mathbf{r}_1 \ldots \mathbf{r}_N) = \prod_{i=1}^{N} u(y_i) \prod_{i<j}^{N} f(r_{ij}) \mathrm{Det}_{\uparrow}\, \phi_\alpha(\mathbf{r}_\beta) \mathrm{Det}_{\downarrow}\, \phi_\alpha(\mathbf{r}_\beta). \tag{2}$$

The Jastrow factor $f(r_{ij})$ is a simplified version of the form used in Ref. 33. The one-body factor $u(y)=\exp(-c_1 y^2)$ is a Gaussian which is used to give an overall correction to the lateral width of the wave function. The single-particle functions are solutions of the noninteracting Hamiltonian, and can be written as

$$\phi_\alpha(\mathbf{r}) = \psi_{\text{ho}}^{l}(y)\phi(x), \tag{3}$$

where $\psi_{\text{ho}}^{l}(y)$ are eigenstates of the harmonic oscillator of frequency $\hat{\omega}_0'$. The single-particle functions $\phi(x)$ can be chosen to enforce the symmetry of the state considered. For simulating the liquid phase, either polarized or unpolarized, we use $\phi(x)=\exp(-ikx)$. The momentum k is consistent with the periodicity of the system: $k=\pm n 2\pi/L$, with n integer. Note that the energy levels of the noninteracting system show a band structure given by $\epsilon_{lk}=\hat{\omega}_0(l+1/2)+k^2/2m$, where l plays the role of the band index. The number N_b of harmonic-oscillator bands filled depends on the density of the system, and must be determined from the Fermi energy of the N particles. In the simulations we assumed that the filling of the bands is the same for the interacting and noninteracting electrons. We checked this assumption by computing the DMC energy for different fillings of the bands, always obtaining the lowest energy for the filling predicted for independent electrons. In order to study the occurrence of a localized phase we implemented another set of single-particle orbitals,

$$\phi_\alpha(\mathbf{r}) = \exp[-(\hat{\omega}_0' + c)y^2]\exp[-c(x-x_j)^2], \tag{4}$$

where x_j are the localization centers located at $y=0$ and distanced by L/N. Because we are considering an antisymmetrized product of such orbitals, this choice does not automatically correspond to constraining an electron around a given lattice site. If the orbitals are overlapping with each other an exchange of electrons is always possible.

The Jastrow parameters appearing in the wave function are optimized following the procedure of Refs. 34 and 35. The c, c_1, and $\hat{\omega}_0'$ are optimized independently. The ground state energy is computed by means of the diffusion Monte Carlo algorithm, in which a population of walkers is evolved in imaginary time according to the Hamiltonian of the system. Some details on the specific implementation of the algorithm can be found in Ref. 36.

IV. RESULTS

Simulations have been performed using different numbers of electrons and at different values of the density, parametrized by the Wigner-Seitz radius r_s. We thoroughly studied finite-size errors that might come from the use of Ewald sums for the potential energy. In order to minimize such errors we chose a rather large number of electrons for our simulations, namely, $N=74$ and $N=98$. At given density, therefore for a given filling of the harmonic-oscillator bands, the consecutive filling of plane-wave shells in the one-dimensional Fermi gas gives rise to a monotonic growth of the kinetic energy, contrarily to what happens in two- and three-dimension. It is possible to observe how this behavior is preserved in the case of the interacting confined system. Test calculations performed with larger numbers of electrons show that the energy differences for numbers of electrons >98 is further decreased, and almost always of the order of the errorbar. This fact allows us to consider the results with $N=98$ essentially converged. The reported energies for smaller size systems can give a sense of the speed and of the order of convergence.

The confinement parameter has been chosen to be $\hbar\omega_0 = 4\ \text{meV} = 0.674\ \text{Ry}^*$, which is representative of typical values used in transport experiments (see e.g., the discussion in Ref. 5). The relevant parameter determining the properties of the wire is the ratio between the gap in the single-particle levels in the harmonic confining potential, and the Fermi energy of the electrons in the longitudinal direction $C_F = 2m\hbar\omega_0/\hbar^2 k_F^2$ (Ref. 37), which in effective atomic units reduces to $32 r_s^2 \omega_0/\pi^2$. Therefore, at least in the strongly one-dimensional regime $C_F \gg 1$, the results should approximately be independent of the specific value of ω_0 and scale as C_F. However, this is not true at high densities, where more than one harmonic-oscillator band is occupied.

In Table I we report the energy per electron computed with $N=74$ and 98 electrons at different values of r_s. The values were computed by using the plane-waves and localized wave function, both for a fully spin-polarized system and for a spin-unpolarized system, in an antiferromagnetic configuration. For the unpolarized liquid phase the number of h.o. bands used in the wave functions is three for $r_s=0.5$, and one for $r_s>1$, while for the polarized liquid phase we fill five bands for $r_s=0.5$, two for $r_s=1$, and one for $r_s>1$. In the localized phase we consider localized orbitals, and we assume that the correct density is reached by varying the parameters of the Gaussians.

As it can be seen, at high densities ($r_s<3$) the ground state is an unpolarized liquid. In particular for $r_s \leq 1$ the C_F parameter is rather small, and the system has a two-dimensional character. For $r_s \geq 5$ the ground state is found to be the spin-polarized, with an energy gap of the order $1\ \text{m Ry}^*$. However, the differences in energy between the polarized liquid (determinant of plane waves) and solid (determinant of Gaussians), and the unpolarized liquid and solid are even smaller. This tiny difference ($<0.1\ \text{m Ry}^*$) might be taken as a conservative estimate of the fixed-node error, suggesting that the energy gap between the polarized and unpolarized phases is robust with respect to changes in the nodal structure. However, it is not possible within our current numerical accuracy to draw a definite conclusion about the relative quality of the two nodal structures.

In Fig. 1 we report the computed energies, together with the fit of the total energy according to the Tanatar-Ceperley[38] functional in the range of 2D densities corresponding to an estimate of the electron density of the wire. As it can be seen, at low values of r_s, the energy of the electrons in the wire becomes closer and closer to that of the equivalent homogeneous 2D system. The discrepancies are due to the approximate way in which the width of the wire is determined. On

TABLE I. Total energy per electron (in Rydberg) for a laterally confined two-dimensional electron gas. (a) unpolarized liquid wave function, (b) localized wave function, (c) polarized liquid wave function, and (d) polarized solid wave function. (*): $N=74$.

N, r_s	0.5	1	2	3	5	7
50 (a)					−0.095596(6)	
74 (a)	−0.5288(4)	−0.36810(5)	−0.26760(3)	−0.19458(3)	−0.09549(1)	−0.026681(7)
98 (a)	−0.5513(4)	−0.36800(8)	−0.26750(3)	−0.19453(2)	−0.09544(1)	−0.026791(7)
50 (b)					−0.09647(1)	
74 (b)	−0.4163(6)		−0.26527(3)	−0.19465(1)	−0.096476(8)	−0.027629(5)
98 (b)	−0.3979(8)		−0.26518(3)	−0.19460(1)	−0.096491(7)	−0.027634(5)
49 (c)					−0.09787(1)	
73 (c)	−0.0424(4)	−0.20522(5)*	−0.21482(1)	−0.19067(1)	−0.097797(6)	−0.028524(4)
97 (c)	−0.0443(4)	−0.20697(8)	−0.21524(1)	−0.19077(1)	−0.097695(6)	−0.028500(4)
49 (d)					−0.09772(1)	
73 (d)				−0.18999(1)	−0.097671(6)	−0.028423(6)
97 (d)				−0.19000(1)	−0.097673(5)	−0.028405(4)

the other hand, the figure clearly displays that in the high-r_s regime the energies of the four phases considered strongly deviates from the 2D value, and tend to collapse on a single value, consistently with the fact that we are approaching an effective 1D regime ($C_F \rightarrow \infty$).

A problem occurring in QMC simulations of quasi-1D systems is the lack of ergodicity due to the extremely low exchange rate between electrons.[30] We tried to assess the existence of this drawback in our 2D simulations. This was achieved both by direct inspection, i.e., by checking the diffusion of close pairs of electrons, and looking at the Monte Carlo mean-square diffusion of the electrons along the wire, estimated by

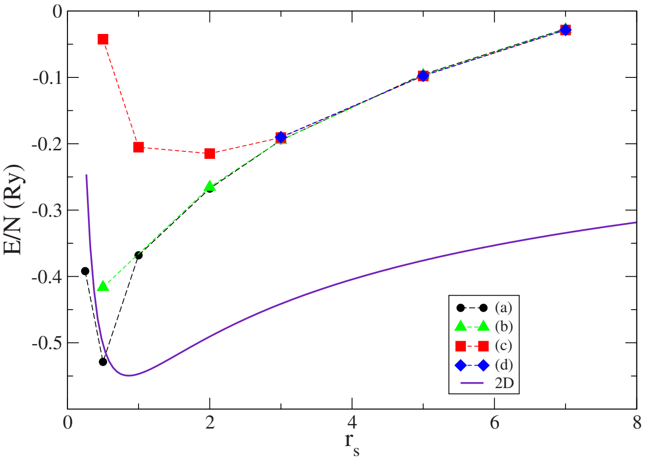

FIG. 1. (Color online) Total energy per electron (in Rydberg) for a laterally confined two-dimensional (2D) electron gas. Dots: unpolarized fluid; triangles: unpolarized crystal; squares: polarized fluid; diamonds: polarized crystal. The full line is the energy of the 2D system at a value of r_s^{2D} estimated from the width of the lateral density of electrons.

$$\langle (\mathbf{x}-\mathbf{x}_0)^2)\rangle = \frac{1}{NM}\sum_{j=1}^{M}\sum_{i=1}^{N}[\mathbf{x}_{j,i}(\tau)-\mathbf{x}_{0,i}]^2, \qquad (5)$$

where $x_i(0)$ and $x_i(\tau)$ (with $\tau = M\Delta\tau$, where $\Delta\tau$ is the time step used in the DMC simulation, $\Delta\tau=0.001$, and $M=175000$) are the x coordinate of the initial and final positions of the electron i after j DMC steps.

In Fig. 2 we report the evaluation of the rms diffusion (in units of a_0^*) as a function of r_s for the four phases considered. For $r_s \leq 2$ the diffusion of electrons is very active. The dependence on r_s (almost linear for the unpolarized liquid phase) is given by the increased size of the wire in the lon-

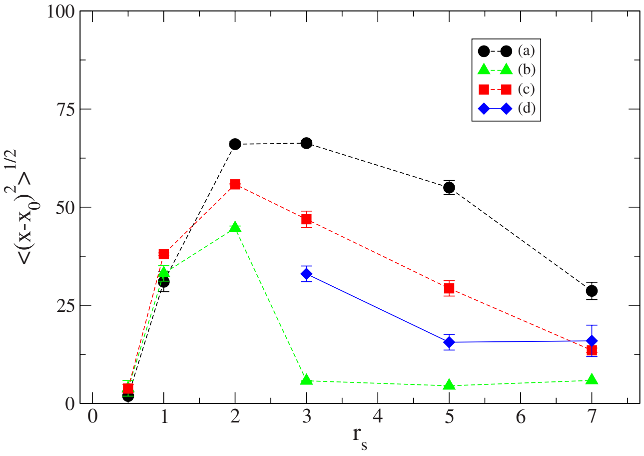

FIG. 2. (Color online) QMC rms diffusion of the electrons in the wire as a function of r_s (in units of a_0^*). The points display the computed diffusion for the unpolarized liquid (dots), polarized liquid (squares), localized (triangles) and polarized solid (diamonds) phases. For small values of r_s the linear growth indicates a diffusion throughout the simulation box. For larger values of r_s the diffusion is increasingly suppressed, as displayed by the decreasing trend of the curves for all the phases considered.

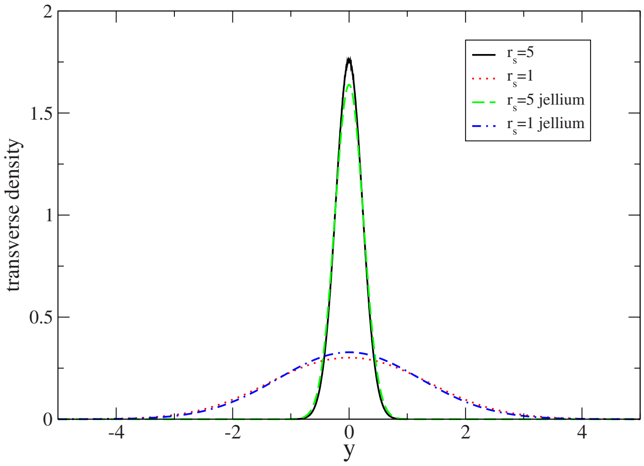

FIG. 3. (Color online) Transverse density in the confined 2D electrons gas. The density computed by DMC is compared with the “jellium” density, i.e., from the density given by the ground state solution of the confining harmonic potential. Curves are given for $r_s\!=\!1$ (dotted and dashed-dotted line), and $r_s\!=\!5$ (full and dashed lines). y is given in units of a_0^*.

gitudinal direction. This is a clear sign of the fact that electrons are allowed to almost freely diffuse for the whole length of the wire. For $r_s \geq 3$ the diffusion ceases to increase. When using localized orbitals, it is clear how the diffusion converges to a constant value much lower than the values seen in the liquid phase, indicating that electrons remain strongly localized around lattice sites.

In Fig. 3 we report the transverse electron density for two different values of r_s and the transverse jellium density. The picture shows how the system becomes effectively narrower with increasing r_s. For $r_s\!=\!0.5$ the system is almost two-dimensional, in agreement with the fact that the energy of the confined system approaches the energy of the 2D system. For lower densities, the effect of the confinement on the energy becomes stronger and stronger.

In Fig. 4 we report the pair-correlation function projected along the longitudinal coordinate, $g(x)$, at $r_s\!=\!5$ computed using the polarized liquid and the localized wave function. The polarized solid-wave function shows the expected oscillations due to the presence of the Gaussians in the Slater determinant. However, it is interesting to notice that the $g(x)$ computed with the polarized liquid wave function (i.e., with plane waves in the longitudinal direction) shows slowly decaying oscillations. The shape of these $g(x)$ suggest that the system tends to form a Wigner crystal even when the wave function does not contain an explicit symmetry-breaking term.

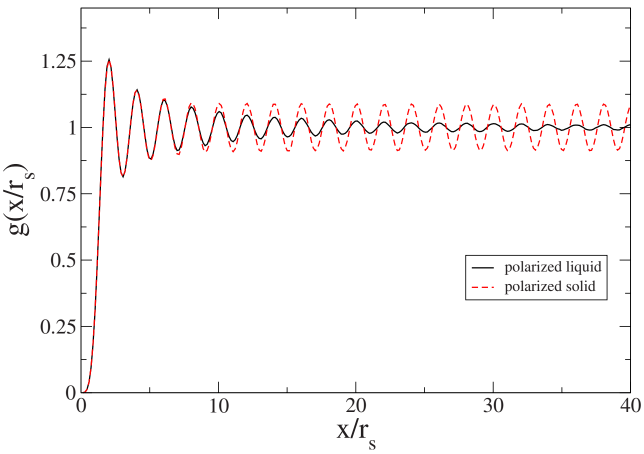

FIG. 4. (Color online) Pair correlation function $g(x)$ at $r_s\!=\!5$, computed using the polarized liquid wave function (solid line) and the solid wave function (dashed line).

V. CONCLUSIONS

We performed a quantum Monte Carlo simulation of a laterally-confined electron gas. In this model, contrarily to quasi-1D models, we can study the occurrence of phase transitions relevant for understanding the anomalies observed in the conductance of quantum nanowires. The occurrence of a polarized and localized phase for $r_s > 3$ suggests that in that limit the conductance of the wire might well be different from the expected value $2e^2/h$. For $r_s < 3$ the ground state is an unpolarized liquid, that, due to the occupation of higher harmonic-oscillator bands, quickly displays a 2D character.

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