Correlation effects in quasi one dimensional electron wires

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We explore the role of electron correlation in quasi one dimensional quantum wires as the range of the interaction potential is changed and their thickness is varied by performing exact quantum Monte Carlo simulations at various electronic densities. In the case of unscreened interactions with a long range 1/x tail there is a crossover from a liquid to a quasi Wigner crystal state as the density decreases. When this interaction is screened, quasi long range order is prevented from forming, although a significant correlation with 4kF periodicity is still present at low densities. At even lower electron concentration, exchange is suppressed and the electrons behave like spinless fermions. Finally, we study the effect of electron correlations in the double quantum wire experiment [Steinberg et al., Phys. Rev. B 77, 113307 (2006)], by introducing an accurate model for the screening in the experiment and explicitly including the finite length of the system in our simulations. We find that decreasing the electron density drives the system from a liquid to a state with quite strong 4kF correlations. This crossover takes place around 22 μm−1, near the density where the electron localization occurs in the experiment. The charge and spin velocities are also in good agreement with the experimental findings in the proximity of the crossover. We argue that correlation effects play an important role at the onset of the localization transition.

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I. INTRODUCTION

It is well known that the effect of interactions in quasi one dimensional (Q1D) systems of electrons, usually called “quantum wires”, is enhanced compared to higher dimensional systems. There are universal properties described by the Luttinger liquid paradigm, the effective low energy theory which applies for strictly 1D models such as spin-charge separation, charge localization, and conductance quantization. However, the microscopic details, such as the width and type of the transverse confinement or the distance and shape of neighboring screening media, can have a large impact on the properties of the Q1D systems, as they are very sensitive to the effective interaction. These systems can be realized in semiconductor structures, where there are elegant experimental studies6,7,8,9,10,11,12 and it is essential to describe the system accurately for a realistic comparison of theory and experiment.

In this paper we study how the thickness, finite size, and screening affect the phase boundaries of some universal features with a particular emphasis on the charge localization and spin properties. We address the issue of how the electron correlation depends upon the microscopic details parametrized in the interaction using ground state quantum Monte Carlo (QMC) methods13,14,15 such as diffusion Monte Carlo (DMC)14,15 and its lattice regularized version16 which are ideal numerical tools to study Q1D systems, since they provide exact results in one dimension. Previous QMC studies regarded the determination of the LL parameters for a Q1D system with screened interactions14,15 and the ground state properties of a model with a long-range Coulomb potential. Here we compare various model interactions in a unified picture, with the final goal of quantifying the role of correlation in the localization transition found by Steinberg et al.6.
charge degrees of freedom is stabilized by the long range tail. The relative importance of the short versus long range correlations is set by the microscopic model of the system. Recently Fogler\textsuperscript{24,25} proposed that a correlated state with very small spin exchange exists for ultrathin wires at densities between the liquid and the quasi Wigner crystal phase. In the limit where the short-range part can be effectively described by an infinite repulsive contact interaction, this state can be related to a noninteracting spinless Fermi system, as in the Tonks-Girardeau gas.\textsuperscript{26} In a one dimensional system of fermions, the coexistence of strong short-range repulsions and very long-range interactions leads to a peculiar state, which Fogler termed a Coulomb-Tonks gas.

In previous theoretical work, quantitatively accurate studies of the liquid-to-crystal one dimensional crossover have been carried out only for inhomogeneous systems, with longitudinal extension controlled by an external confinement, and where the finite (and very small) size allows one to solve the problem by means of exact diagonalization.\textsuperscript{27-29} However, the broken translational symmetry leads to quite different properties, particularly in the charge and spin density profiles.

From the experimental side, technological advances in the preparation of cleaved edge overgrowth samples have enabled tunneling measurements between two high mobility parallel wires, which probe striking features like the spin-charge separations in the excitation spectra.\textsuperscript{22} In a recent extension of the tunneling experiments, Steinberg et al.\textsuperscript{6} applied a gate to the upper wire in order to tune its electron density by charge depletion. Below a critical threshold, measurements revealed a dramatic transition which can be interpreted as the onset of localization in the wire. Although it is believed that the transition is mainly driven by electron-electron interaction effects as the liquid phase is in a ballistic regime, so far there is no agreement between the critical density predicted by theory and the actual experimental value. Some features of the experiment, like the fringes of the differential conductance in the liquid phase and the first two peaks of the tunneling current in the localized phase, have been explained in an independent particle picture and at the mean field level.\textsuperscript{20} The LL theory has been applied to describe the general features of the tunneling current in the Wigner state by assuming a spin incoherent regime.\textsuperscript{31} However it is unclear at which density the spin degrees of freedom become incoherent, as the spin velocity measured in the experiment is in disagreement with previous numerical estimates. Another open issue is related to the fact that only a small fraction of electrons take part in the localized state. It is clear that an accurate microscopic description of the experimental situation is necessary to account for all these features. In our study we include the most important details such as an accurate screening and the effect of the finite size of the wire to correctly describe and understand the physics underlying the experiment.

Throughout the paper we use units of the effective Bohr radius $a_0^* = \frac{\hbar^2}{m^*e^2}$ for length and the effective Rydberg $\text{Ryd}^* = \frac{\epsilon^2}{2m^*e^2}$ for energy where $\epsilon$ is the dielectric constant of the embedding medium and $m^*$ is the effective electron mass.

The paper is organized as follows: in Sec. II we present results for a quasi one dimensional electron gas (1DEG) with long range $(1/x)$ interactions for different densities $\rho = \frac{1}{\pi r_s b}$, and thicknesses. We carefully study the liquid-to-quasi-crystal crossover by varying the Wigner-Seitz radius $r_s$ which sets the relative importance of the kinetic energy and the interaction. By means of QMC techniques, we also study the charge compressibility and the spin susceptibility in order to analyze the interplay between the charge and spin properties of the wire. The effect of the wire’s thickness on the crossover and the spin properties is taken into account by performing simulations with three different wire widths. In Sec. III we compare the unscreened $1/x$ potential with an interaction screened by a metallic plane. In Sec. IV we interpret the localization transition found in the series of two wire tunneling experiments by studying the evolution of liquid-to-crystal correlations in a finite wire with interactions effectively screened by another parallel wire. We make a comparison between the finite system and the corresponding homogeneous infinite system interacting with the same potential. We also show the agreement between our model and the experiment. Finally in Sec. V we summarize our results and comment on possible refinements to our calculations.

II. UNSCREENED COULOMB INTERACTIONS

We study a system of electrons interacting via the Coulomb $(1/x)$ potential which are confined to one dimension by a harmonic potential in the transverse direction $V(x) = \frac{r_s^2}{x^4}$, where $b$ tunes the thickness of the wire. This system was previously studied using QMC by Casula et al., and here we follow the conventions used in that work.\textsuperscript{32} We integrate over the transverse degrees of freedom, which is a good approximation when the density of electrons in the wire is low ($r_s \gg \pi b/4$), and hence the longitudinal energy scale is small compared to the excitation energies related to the perpendicular motion. This integration yields an effective one dimensional interaction: $V_b(x) = \frac{\sqrt{\pi}}{b} \exp \left( -\frac{x^2}{4b^2} \right) \text{erfc} \left( \frac{ix}{2b} \right)$, which has a long range $1/x$ tail. The thickness $b$ of the wire controls the short-range behavior of the potential, which is finite at the origin ($V(0) = \sqrt{\pi}/b$). Since the crossover between the short and long range behavior is at $x \approx b$, for smaller $b$ the repulsion is stronger as the particles approach each other.

In this work we have chosen to study three different thicknesses, $b = 1, 0.1$, and 0.0001. The first two values correspond to typical experimental thicknesses for semiconductor quantum wires, whereas the last one is chosen to explore the ultrathin limit as studied analytically by
tem, we first analyze the static structure factor in the real space as the potentials have a shorter range. In the latter case, the sum over the images has been done numerically with the long range potential included in the trial wave function. A particular diffusion Monte Carlo (LRDMC) method is particularly suited to the simulation of one dimensional fermions. Indeed, the well known \textit{“sign problem”} does not affect these calculations as the nodes are fully determined by the points of coincidence between the electrons and therefore are exactly included in the trial wave function $|\Psi_T\rangle$. Since the final DMC or LRDMC distribution is the product of the true ground state and the trial wave function, some observables such as the density and the structure factor are determined using the forward walking technique in order to generate unbiased expectation values.

We simulate an unpolarized wire with $N$ electrons subject to periodic boundary conditions (PBC). The trial wave function is written in the Slater-Jastrow form

$$ \Psi_T = D^U D^D \exp \left( - \sum_{i<j} u(x_{ij}) \right), \tag{1} $$

where the Slater determinants for up and down spin electrons read

$$ D^\sigma(x_1^\sigma, \ldots, x_N^\sigma) = \prod_{1 \leq i < j \leq N^\sigma} \sin \left( \frac{G}{2}(x_i^\sigma - x_j^\sigma) \right), \tag{2} $$

with $G = 2\pi/L$, and $L = 2\pi N$ the length of the simulation cell. We follow Ref. 36 to determine the Jastrow function $u(x)$. Its Fourier components are

$$ 2\rho\tilde{u}(k) = -S_0(k)^{-1} + \sqrt{S_0(k)^{-2} + 2\rho\tilde{V}_b(k)/k^2}, \tag{3} $$

with $S_0(k) = (k/2k_F)^2 \theta(2k_F-k)+\theta(k-2k_F)$ the structure factor of a noninteracting 1DEG, $\rho = \frac{1}{2\pi}$ the density, and $\tilde{V}_b(k)$ the Fourier transform of $V_b(x)$. To reduce the finite size effects in our simulation we use the Ewald technique to sum our potential as discussed in detail in Ref. 18. This approach has been used to study the infinite wire with the long range potential $V_b(x)$, and also the screened potentials described in the next Sections. In the latter case, the sum over the images has been done numerically in the real space as the potentials have a shorter range.

To reveal the presence of charge ordering in the system, we first analyze the static structure factor $S(k) = \frac{1}{N} \langle \rho(-k)|\rho(k) \rangle$, where $\rho(k) = \sum_{i} e^{ikr_i}$ are the Fourier components of the electron density. At high density the structure factor is very similar to the mean spherical approximation (MSA) prediction $S_{\text{MSA}}(k) = S_0(k)/(1 + 2\rho\tilde{u}(k)/k^2)$ as expected (see Fig. 1), since in the limit $r_s \rightarrow 0$ the MSA becomes exact. Specifically, there is no peak at $4k_F$ up to $r_s = 0.5$ ($r_s = 0.2$) for $b = 0.1$ ($b = 0.0001$), namely there are no correlations with the mean interparticle spacing (Fig. 2). As the density decreases, a peak develops at $4k_F$. This peak is a necessary feature for a one dimensional quasi Wigner crystal and it is absent in the MSA prediction which has no structure at $4k_F$. For $b = 0.1$ we carried out simulations with up to 450 particles for $r_s = 0.5$ and $r_s = 0.75$, to check the convergence of the $S(k)$ in the liquid regime close to the onset of the $4k_F$ charge correlations (Fig. 2).

The scaling of the height of the $4k_F$ peak of $S(k)$ with the number of particles (reported in Fig. 3 for $b = 0.1$) highlights the features of a liquid-to-quasi crystal crossover. When the peak is absent there is no significant dependence of the $S(4k_F)$ value as a function of system size, however where there is a peak in the structure factor at $4k_F$, its scaling is sub-linear, signaling a quasi-long range order (linear scaling would indicate a true Wigner crystal). The points in Fig. 3 are fit very well by a functional form obtained from the charge-charge correlation function derived by Schulz in the LL framework with long range interactions,

$$ \int_{C_0}^L dx \exp(-4k_F x) \langle \rho(0)\rho(x) \rangle = aL \exp(-4c \sqrt{\log L} + b), \tag{4} $$

where we explicitly include the dependence on the system size $L$ by taking the Fourier transform over the simulation cell. The short-distance cutoff $C_0$ is introduced because the LL theory provides only the asymptotic behavior for $\langle \rho(0)\rho(x) \rangle$. Further logarithmic corrections could be included in Eq. 4 but we take just the leading order expansion, which should be the most relevant for the system sizes computed here. One would need much larger systems which are beyond our current numerical capabilities to resolve further corrections. The bosonization formalism gives a parameter dependent scaling for the $4k_F$ component of $\langle \rho(0)\rho(x) \rangle$ which is left undetermined in the LL theory, and depends on the details of the interaction. At high densities there is no peak in the structure factor and the electron gas is liquid (Fig. 2). Consequently, there is no finite size dependence at $4k_F$ and the parameter $a$ undetermined in the LL theory is zero.

We also determine the charge compressibility $\chi_\rho$ and the spin susceptibility $\chi_\sigma$ of the electron gas by using two techniques in our calculations. The first is to apply the definition of those quantities as the reciprocal of the second derivative of the total energy with respect to the density $r_s$ or the polarization $\zeta$. Our QMC calculations provide measurements of the total energy, so these derivatives can be taken by fitting our data with a suitable functional form. The error in such a determination comes from both the statistical uncertainty in the calculations and the constraint represented by the choice of the fitting function. As a technical detail, it is also necessary to extrapolate the energy to the thermodynamic limit which can be a costly proposition. Moreover a functional form which includes the dependence on both density and
polarization has not been provided yet. Nevertheless, we use the parametrization in Ref. 18, which holds for a system with fixed polarization $\zeta$ and depends only on $r_s$ to compute the charge compressibility and validate the second method to evaluate $\chi_\rho$ and $\chi_\sigma$.

The other method we use to compute these quantities is to calculate the momentum resolved excitation energies of the system, and exploit the sum rules which exactly relate the collective modes of the long wavelength spectrum with $\chi_\rho$ and $\chi_\sigma$. Gold and Calmels\cite{41} found that

$$\omega_\rho(k \to 0) = v_F |k| \sqrt{\rho_F V(k \to 0) + \chi_0 \over \chi_\rho}, \quad (5)$$

$$\omega_\sigma(k \to 0) = v_F |k| \sqrt{\chi_0 \over \chi_\sigma}, \quad (6)$$

where $\omega_\rho(k)$ ($\omega_\sigma(k)$) is the energy of the lowest charge (spin) excitation with momentum $k$, $\rho_F$ is the density of states of the free electron gas at the Fermi energy, and $\chi_0 = 16r_s^3/\pi^2$ is its compressibility.

FIG. 1: (Color online) Structure factor for $b = 0.1$ (upper panel), and $b = 0.0001$ (lower panel), computed for a system with 78 electrons. The QMC (points) and MSA (solid lines) structure factors are reported for different densities ($r_s$). Also the noninteracting spinless fermion (NSF) structure factor is drawn (solid black line) for comparison.

FIG. 2: (Color online) Detail for the structure factor near $4k_F$ for $b = 0.1$, computed for $N = 182$ and $N = 450$ at two densities ($r_s = 0.5$ and $r_s = 0.75$) in the proximity of the crossover from a liquid to a quasi-crystal.

FIG. 3: (Color online) Scaling of the $4k_F$ component of the structure factor with respect to the number of particles. The scaling is reported for various densities with $b = 0.1$. The lines are the best fit of the function in Eq. (4) given by the LL theory.

In order to find out the lowest energy states of a given momentum $k$ we employ a method proposed by Ceperley and Bernu\cite{42} which is a generalization of the transient estimate used in the projection Monte Carlo (DMC or LRDMC) framework. This method is based on the idea that it is possible to compute the excitation spectrum of a system in a direct and variational way by projecting the initial basis functions to their lowest energy state with the given symmetry. In our case the basis set is the Feynman ansatz\cite{42} i.e. $\rho(k)|\Psi_0\rangle \forall k$ for the charge excitations and $\sigma(k)|\Psi_0\rangle \forall k$ for the spin excitations, where $\sigma(k) = \sum_j \sum_\delta \sigma e^{ikr_j}$ is the Fourier transform of the spin density. In the following we assume to work with the charge excitations, but the same applies for $\sigma(k)$. Since the basis set is orthogonal, the method in Ref. 42
is greatly simplified, as every k component is decoupled. For each k, we have to calculate
\[ \langle \Psi_0 | \hat{\rho}(k, \tau) \hat{H} \rho(-k, 0) | \Psi_0 \rangle = \sum_i \epsilon_i^k A_i^k e^{-\tau(\epsilon_i^k - E_0)}, \]
where \( \hat{\rho}(k, \tau) \) is written in the Heisenberg representation with imaginary time evolution, \( |\Psi_k^i\rangle \) is the \( i \)th excited state with momentum \( k \), \( \epsilon_i^k \) is its energy, \( A_i^k \) = \[ |\langle \Psi_0 | \rho(-k) | \Psi_i \rangle|^2 \] is the spectral weight of the eigenvalue expansion, and \( E_0 \) is the ground state energy. For large \( \tau \) the ratio in the above Equation will converge to the lowest energy \( \epsilon_0^k \) of a given \( k \), provided \( A_i^k \) is non zero. Another limitation is given by the exponentially small denominator, which will exponentially increase the statistical noise of the estimate as the projection time increases. Both the numerator and denominator in Eq. 7 are evaluated by means of the forward walking procedure based on the DMC or LRDMC sampling. Indeed, for large enough \( \tau \) the LHS of Eq. 7 can be rewritten as
\[ \frac{\int dr_1 dr_2 \rho(-k)G(r_1, r_2, \tau)E_L(k, r_2)\rho(k)P(r_2)}{\int dr_1 dr_2 \rho(-k)G(r_1, r_2, \tau)\rho(k)P(r_2)}, \]
where \( E_L(k, r) = \frac{\hat{H}(k, r)}{\rho(k)\Psi_T} \) is the local energy of \( \rho(k) |\Psi_T\rangle \), \( P(r) = \Psi_T(r)\Psi_0(r) \) is the QMC mixed distribution, and \( G(r_1, r_2, \tau) = \Psi_T(r_1)\langle r_1 | e^{-\tau H} | r_2 / \Psi_T(r_2) \) is the importance sampled Green’s function.

Because the excitation energies \( \omega(k) = \epsilon_0^k - E_0 \) are computed relative to the ground state energy \( E_0 \), there is a cancellation of errors since the sample generated to compute \( E_0 \) and \( \epsilon_0^k \) is the same. Therefore a modest size calculation is enough to get converged energies. The convergence with the propagation time can be more difficult to obtain. However, for the long wavelengths \( \rho(k) |\Psi_0\rangle \) is a good approximation to the lowest excited state with momentum \( k \) and the energies can be determined easily with a short projection time \( \tau \). When the small \( k \) range of energies is fit to the form in Eqs. 3 and 6 \( \chi_\rho \) and \( \chi_\sigma \) are determined. The results for the charge compressibility obtained with this method agree with the second derivatives of the total energy in all cases we have made the comparison, as is shown in Fig. 4.

The knowledge of \( \chi_\rho \) and \( \chi_\sigma \) can shed more light on the properties of the liquid-to-quasi-crystal crossover. By looking at the charge compressibility (Fig. 4), it is apparent that the role of the electron correlation is becoming increasingly important in the proximity of the crossover, where there is significant discrepancy between the Hartree-Fock (HF) and QMC values of \( \chi_\rho \). In particular, the correlation makes the system softer than the HF, which is consistent with a more pronounced localization of the electrons. At even lower densities the charge compressibility of the unpolarized system is approaching that of a fully polarized (or spinless fermion) gas. The difference between the two is going exponentially to zero, and they almost overlap for \( r_s > 4 \) (with \( b = 0.1 \). This means that the energy of the spin excitations is getting smaller and smaller as the density decreases. This feature is revealed by the inverse spin susceptibility \( \chi_\sigma \). The \( \chi_\sigma / \chi_\rho \) ratio is plotted in Fig. 5. This value becomes exponentially small at low densities, where it is difficult to get a statistically accurate QMC estimate, since the sampling of the spin is “frozen” by the presence of quasi nodes (pseudo nodes) between unlike spin electrons. The strong interaction makes the electrons to repel each other at short-range, and the corresponding wave function is very small at the coalescence points of electrons with opposite spin. Consequently the spin flip rate in the QMC sampling becomes small, and the efficiency decreases. However the charge properties do not seem to be affected by this slowing-down. The physical reason for the quasi nodes will become even more apparent in Sec. III when we will discuss the Tonks-Girardeau physics of the screened wire.

In the low density regime where exact Monte Carlo sampling becomes difficult the WKB approximation is useful for determining the dynamical properties of the electron gas. Following the example of Matveev we use the WKB approximation to determine the rate at which two electrons exchange by calculating the energy barrier that they must overcome. Although fluctuations prevent the formation of a Wigner crystal, the equilibrium positions of the electrons are assumed to be equally spaced with periodicity \( 2r_s \). Central to the accuracy of this approximation is the fact that at low densities the tunneling is dominated by the effect of the potential, and the statistics can be ignored. Furthermore, all electrons are treated as uncorrelated except for a single pair which is allowed to exchange. In contrast to Matveev’s approach we assume that the other electrons are distributed about their equilibrium positions according to the harmonic approximation with a Gaussian spread instead of being fixed delta function point particles. Taking the initial positions of the two exchanging electrons to be at \( x = 0 \) and \( x = 2r_s \), they feel a static potential given by
\[ V_{WKB}(x) = \sum_{n \neq 0} \int_{-\infty}^{\infty} \rho(y)V(x - 2nr_s + y)dy, \]
where \( \rho(y) = \sqrt{\alpha / \pi} \exp(-\alpha y^2) \) is the equilibrium charge density of the non exchanging electrons and \( V(x) \) is the interparticle potential. The harmonic approximation gives \( \alpha = \sqrt{m^2 W(x) / 2} \), where \( W(x) \) is the potential at a given lattice site due to an infinite array of electrons spaced as \( 2r_s \).

At low densities the electrons behave as a spin chain obeying the Heisenberg Hamiltonian were the spin flips are mediated by an exchange of nearest neighbor electrons, so the spin susceptibility can be determined from the energy barrier computed within the WKB approximation by analogy with the Heisenberg Hamiltonian in 1D as shown by Matveev. The spin velocity of the equivalent Heisenberg spin chain can be found from the Bethe ansatz solution, yielding \( v_\sigma = \pi J r_s / 2 \) where \( J \) is the size of the energy barrier in the WKB approximation. This gives the susceptibility through Eq. 6.
Where the density is large enough that QMC reliably samples the spin exchanges the spin susceptibility computed using the forward walking techniques agrees well with the WKB estimate only after the smearing of the electron sites given by the harmonic approximation. It is therefore important to use the potential in Eq. 8 to have an accurate estimate of the exchange at intermediate densities. This agreement and the fact that the dynamical many-body corrections to the WKB estimate are very small at low density\(^7\) justify the use of WKB for dilute systems where it is difficult to extract information from the QMC calculations. In addition, the exponential decay of \(v_s\) versus \(\sqrt{r_s}\) obtained in this way is in agreement with previous results\(^{44,47,48}\) for potentials where they can be compared.

Fig. 4 summarizes our findings for the unscreened wire. The liquid-to-quasi-crystal crossover is shifted to higher densities for thinner wires, while the spin susceptibility is always significantly different from zero in the crossover region for the values of the confinement taken into account. The smallest \(b\) we studied (\(b = 0.0001\)) corresponds to one of the thinnest confinements realized experimentally\(^{32,33}\). The spin exchange is still sizable in the crossover region due to the not-so-long localization length of the electrons and not-so-thin width of the wire. Therefore, in our study we did not find any signature of the Coulomb-Tonks gas phase in between the liquid and quasi Wigner crystal, which was claimed by Fogler for ultrathin wires\(^2\). However, the structure factor plotted in Fig. 1 reveals the tendency for electrons to approach the noninteracting spinless fermion behavior (the limit where the Coulomb-Tonks gas picture holds) as the wire width decreases. The fundamental difference with respect to the noninteracting spinless picture is the pronounced peak at \(4k_Fr\), which characterizes the Coulomb long-range interactions at low density.

**III. SCREENED INTERACTIONS IN GATED WIRES**

The primary interest of this paper is to model a quantum wire formed in a semiconducting nanodevices. In that case there is almost always a metallic gate that screens the long range \((1/x)\) potential. To see the changes that such a gate would cause, we introduce a perfectly conducting metal plane parallel to the wire located a distance \(R\) away. Using the electrostatic method of images the potential is constructed by assuming that a wire is placed at a distance \(2R\) from the original one with the same particle distribution but opposite sign. The equation for this potential is

\[
V(x) = \int \int d\vec{r} d\vec{r}’ \frac{\rho_0(\vec{r})\rho_s(\vec{r}’)}{\sqrt{(\vec{r} - \vec{r}’)^2 + x^2}} - \int \int d\vec{r} d\vec{r}’ \frac{\rho_0(\vec{r})\rho_s(\vec{r}’)}{\sqrt{(\vec{r} - \vec{r}’ - 2\vec{R})^2 + x^2}}
\]

\[
= V_0(x) - V_{int}(x, R)
\]

where \(\vec{r}\) and \(\vec{r}’\) are transverse vectors, \(\rho_s(\vec{r}) = \frac{1}{b\sqrt{2\pi}} \exp\left(-\frac{\vec{r}^2}{2b^2}\right)\) is the ground state charge distribu-
tion of a two dimensional harmonic oscillator with the wire’s confining potential: \( V_{\text{wire}}(r) = \frac{U}{r} \). The first integral gives the effective unscreened inter-particle potential \( V_0(x) \) described in the previous section and the second one is the potential due to the image charge on the screening wire: \( V_{\text{int}}(x, R) \).

The quasi Wigner crystal correlations derived by Schulz\(^{23}\) apply only when the interaction is long range (1/x). In the case of the screened interaction above the potential decays as \( 4R^2/x^4 \) at large distances, so a simple scaling argument shows that the Wigner crystal correlations should be absent at very low densities. Indeed, if \( r_s > 8R^2/\pi \) the typical kinetic energy of the electrons, the Fermi energy \( E_F \), is larger than the potential energy computed at the mean interparticle distance \( (2r_s) \). At these low densities Matveeva\(^{23}\) has pointed out that it is possible to map the screened short-range interaction into a repulsive contact potential

\[
V(x) = U \delta(x),
\]

where the constant \( U \) is chosen so the delta function potential and the screened one have equal transmission coefficients. On the other hand, in the density range \( 1 < r_s < 8R^2/\pi \) the 1/x shoulder of the potential can induce \( 4k_F \) correlations, which are strong but not strong enough to stabilize any sort of quasi-order. Calculations of the finite size scaling of the \( 4k_F \) peak of the structure factor for \( b = 0.1 \) and \( R = 200 \) show the saturation of its height for \( N \gtrsim 100 \), and so demonstrate the absence of the quasi Wigner crystal correlations when screening is introduced despite quite a large distance to the metallic gate (Fig. 6). Only in the limit of \( R \to \infty \) does one recover the unscreened potential and the possibility for a quasi long-range charge order.

FIG. 6: (Color online) Scaling of the \( 4k_F \) component of the structure factor with respect to the number of particles for \( b = 0.1 \), and \( r_s = 4 \). For comparison, the scaling is reported for the unscreened \( V_0 \) interaction, and the screened potential in Eq. (11) with \( R = 200 \).

The lack of the quasi Wigner crystal state does not change the crossover to the spinless fermion physics present in the unscreened system. Even though the quasi long-range charge order is absent at low densities, the charge compressibility still approaches that of a gas of spinless fermions as the density decreases. This approach can seen in Fig. 4. It is therefore clear that the spin crossover does not depend on the long-range correlations.

In fact, this crossover can be reproduced by a system of electrons interacting via the delta function interaction in Eq. (11) where the constant \( U \) is large, an interaction that has no long-range piece whatsoever.

The low density limit with screened interactions is particularly interesting as the screening introduces a new feature. At low densities the electron-electron repulsion at short range makes exchanges between electrons virtually impossible, corresponding to the limit \( U \to \infty \). As a result for the ultrathin wire with strong screening \((b < 1 \text{ and } r_s > 8R^2/\pi)\), the mapping of the interaction to the potential in Eq. (12) becomes exact. In this situation not only do the electrons behave as spinless fermions, but the charge velocity approaches that of noninteracting spinless fermions \((v_F = 2eF)\). This is analogous to the case of bosons with infinite repulsive contact interactions, (or impenetrable particles) where the system can be mapped into a noninteracting Fermi gas.\(^{25}\) The impenetrable Bose system is often called a Tonks-Girardeau gas. In our case the situation is analogous, namely the fermions become impenetrable due to an effective infinite contact repulsion, and so they behave as they were noninteracting and spinless. We refer to this behavior as Tonks-Girardeau regime. One of its features is the presence of nodes in the wave function at the coalescence of unlike spin pairs. This is the extreme case when the pseudo nodes that complicate the ergodicity of Monte Carlo calculations at low density as reported in Sec. II become actual nodes.

While this effect has been discussed in the literature,\(^{26,35,44}\) our work provides quantitative predictions for the onset of the noninteracting spinless behavior. Fig. 7 shows the charge velocity in the limit of low density for different values of the screening in the thinnest wire we studied \((b = 0.0001)\). We found that in order for the Tonks-Girardeau behavior to manifest itself, the distance to the gate \( R \) must be less than 0.1 and the density must be lower than \( r_s = 1 \). For \( R \) larger than 0.1, at low density the charge velocity does not converge to the noninteracting spinless fermion limit \((2v_F)\), but saturates at a larger value.

It is possible to see the transition of the screened electron gas to the noninteracting spinless fermion behavior more directly by analyzing the static structure factor, as was done in the unscreened case. In Fig. 8 the \( S(k) \) is plotted at different densities for the ultrathin wire with \( b = 0.0001 \) and gate located at \( R = 0.1 \) from the wire. Contrary to the case of the unscreened wire (Fig. 1 lower panel), at low densities the peak at \( 4k_F \) is absent and the structure factor approaches that for noninteracting spinless fermions quite closely. Notice that at the same time the charge velocity approaches the value of \( 2v_F \) (see Fig. 7).
IV. LOCALIZATION TRANSITION IN TWO PARALLEL GaAs WIRES

Quasi one dimensional systems can be realized in GaAs/AlGaAs heterostructures by means of various techniques. One such technique being cleaved edge overgrowth, which has been applied recently to build an experimental setup with two parallel wires so that it is possible to observe momentum resolved tunneling from one to the other. In this series of experiments both the energy of the tunneling electrons and their momentum could be tuned by changing the relative chemical potential and the applied magnetic field. This setup allows the dispersion relations of each wire to be probed in a quite straightforward manner. Steinberg et al. further explored how this tunneling is affected by a gate that depletes the density of the electrons in the upper wire. They found that as the density is decreased there is a marked transition in the tunneling interpreted as a transition from a liquid to a localized state.

In the experiment, the center to center distance between the two wires is $R = 31\text{nm}$. The upper wire is $2\mu\text{m}$ long and $20\text{nm}$ wide. It is the probe to study the electron localization. The electrons tunnel from the lower wire, which has a width of $30\text{nm}$ and is taken to be infinitely long. This is also a screening medium for the upper wire. The system is fabricated out of GaAs for which $\epsilon = 13.1$ and the effective electron mass is $m^* = 0.067m_e$. This gives an effective Bohr radius $a_0^* = \frac{\hbar^2}{m^*e^2} \approx 10 nm$. For the experiment in question the electron density in the lower wire is around $60 \mu m^{-1}$, which corresponds to $r_s = 0.83$ in $a_0^*$ units, while in the upper wire the density is varied by tuning the gate voltage $V_G$. The effect of $V_G$ on the lower wire is very small and can be neglected.

The results presented in the previous section offer an avenue to explore the role of the electron correlation in the transition observed in the experiment. As the density in the wire decreases the strength of the potential increases relative to the kinetic energy. One effect of this increased relative strength is that exchanges between the electrons are suppressed, causing the system to crystallize. To better quantify the importance of this effect in the experimental system, in this section we take into account a more realistic potential, assuming the electrons are screened by the lower wire instead of an infinite metallic gate. To construct this interaction we neglect the correlation between the wires and treat the screening effects coming from the electrons in the lower wire within the linear response theory. We write the potential in Fourier space

$$V(k, R) = V_b(k) + V_{int}(k, R)\chi(k) V_{int}(k, R), \quad (12)$$

where $V_b(k)$ and $V_{int}(k, R)$ defined in Eq. [10] are the intra- and inter- wire potentials respectively. $V_{int}(k, R)$ is evaluated by assuming that the thickness of the two wires is the same (and equal to the upper wire). This significantly simplifies the form and the calculation of the inter-wire interaction. $\chi(k)$ is the static density-density response

The same study was repeated for the wire with $b = 0.1$. Here the short-range behavior of the potential is much less repulsive than in the $b = 0.0001$ case and the same value $R$ for the screening. The result of this is that the charge velocity does not converge to $2v_F$ even for a gate as close as $R = 0.1$, which equals the width of the wire and thus represents the geometric limit of validity for the uncorrelated inter-wire interaction. Therefore for $b = 0.1$ and thicker wires, whose widths are realizable in semiconducting nanostructures, we did not find the Tonks-Girardeau behavior in our calculations.

FIG. 7: (Color online) Asymptotic large $r_s$ values of the charge velocity in units of $v_F$ vs. inverse screening length for ultrathin wire ($b = 0.0001$) from $R = 0.05$ to $R = 5$. In the inset we report the full dependence of the charge velocities on $r_s$ at different $R$.

FIG. 8: (Color online) Static structure factor for the screened wire with $b = 0.0001$ and $R = 0.1$, plotted for three values of the density, $r_s = 0.2, 0.4$ and 0.8. The solid lines correspond to the MSA prediction for each density, and the black line is the structure factor for noninteracting spinless fermions (NSF).
function of the lower wire, taken in the random phase approximation (RPA):

\[
\chi_{RPA}(k) = \frac{\chi_0(k)}{1 - V_b(k)\chi_0(k)}
\]

(13)

where \(\chi_0(k) = \frac{1}{\pi} \ln \left| \frac{k - 2k_F}{k + 2k_F} \right| \) is the static response function for a one dimensional noninteracting Fermi gas, and \(b'\) is the width of the lower wire. The experimental geometry sets the parameters in our quasi one dimensional interaction \(V(k, R)\). The confinement potential for the upper wire is chosen so that the electrons are constrained to be inside the 10µm thick wire. Specifically, we require the radial root mean squared displacement is equal to the lithographic thickness yielding \(b = 0.707(\approx 1/\sqrt{2})\) for the upper wire. The choice of confinement also agrees well with the experimental observation that a second mode becomes populated at \(n = 80\mu m^{-1}\). Similarly, the lower wire’s thickness is given by \(b' = 1.061(\approx 1.5/\sqrt{2})\). The distance between the wires is \(R = 3.0\), while the Fermi momentum in the RPA response function for the lower wire is set by the density \(r_s = 0.83\).

Our screened potential in Eq. (12) is similar to that used by Fiete et al. who chose a perfect metal response function which is valid when the screening wire is at very high densities. Here we use the RPA which depends on the experimental density of the lower wire through the value of the Fermi momentum \(k_F\). We notice that our screened potential equals that in Ref. [51] at \(k = 2k_F\) and in the limit of small \(k\), namely the long-range tail is the same, decaying approximately as \(1/x\).

We first analyze the homogeneous system and then explicitly include a longitudinal confinement in our simulations to quantify the finite-length impact on the properties of the system, and more closely reproduce the experimental situation. In the homogeneous system of electrons interacting via the potential in Eq. (12), we observe the appearance of a 4\(k_F\) peak in the \(S(k)\) around \(r_s = 2.2\). As shown in Fig. 9 it is clearly visible for \(r_s > 2.6\), whereas no peak is discernable for \(r_s \leq 1.9\). This crossover is similar to that found for long range \(1/x\) interactions. However, the important difference here is that the quasi long-range order is not present in this case. Indeed, we have made a systematic study of the scaling with size, and the height of the peak converges to a finite value in the thermodynamic limit for all densities taken into account. This behavior is consistent with the decay of the screened interaction which is faster than \(1/x\). Therefore, the crossover is between a high-density liquid to one with strong 4\(k_F\) correlations, whose onset can be related to the transition occurring in the experimental system.

The above treatment of the upper wire as infinite and homogeneous can be improved to resemble the experiments more closely. In the study of the 1DEG there are strong effects due to any perturbation that breaks the translational invariance of the system. For instance, Tserkovnyak et al. showed that the asymmetry in the oscillations of the conductance as a function of the momentum transferred between the two wires can be explained at the WKB level by having a soft confinement potential for the upper wire. In a later paper they accurately determined the functional form of the longitudinal confinement by fitting its parameters to reproduce the period of those oscillations as a function of the magnetic field applied to the sample. The potential that provided a good fit to their data reads

\[
V(x) = E_F \left( \frac{2x}{L} \right)^8,
\]

(14)

where \(E_F\) is the Fermi energy of the upper wire, and \(L\) is approximately 1.5 times the lithographic length of the upper wire, namely \(L = 300\) in \(a_0\) units.

We used the above potential together with the interparticle potential in Eq. (12) to study the effect of the confinement on the transition. Although in principle diffusion Monte Carlo yields an unbiased ground state energy in one dimension even for a confined system, (the nodes being exactly determined by the coalescence conditions just as in the infinite homogeneous wire) in practice it is necessary to improve the guidance wave function to reduce the variance of our estimates. The Jastrow factor used in the homogeneous system (Eq. 8) is replaced by a more sophisticated factor including one-, two-, and three-body terms, fully optimized by means of the stochastic reconfiguration (SR) algorithm while the Slater part is kept the same as in Eq. 4. The one-body Jastrow \(\exp(J_1)\) is needed to localize the electrons in the finite

![FIG. 9: (Color online) Static structure factor for a homogeneous wire with \(b = 0.707\) interacting with the effective potential in Eq. (12) which includes the screening by another homogeneous wire with \(r_s = 0.83\), \(b = 1.061\), and \(R = 3\). The structure factor is plotted for several values of the upper wire density, with \(r_s\) ranging from 1.7 to 9.4. The calculations have been converged to the thermodynamic limit, requiring \(N = 62\) for \(r_s \leq 3.0\) and \(N = 78\) subject to periodic boundary conditions for \(r_s = 4.6\) and 9.4.](image-url)
system. It reads
\[ J_1 = \sum_{i=1}^{N} (-\alpha x_i^4 - \beta x_i^6), \tag{15} \]
where \( \alpha \) is a free parameter and \( \beta = \sqrt{E_{\text{a}}(2/L)^2}/5 \) is fixed to cancel the contribution of the potential to the local energy at the leading order in the large distance expansion. The two-body \( \exp(J_2) \) and three-body \( \exp(J_3) \) Jastrow factors are given by
\[ J_2 = \sum_{\langle i\sigma\rangle < \langle j\sigma'\rangle} u_{2}^{\sigma\sigma'}(x_{ij}), \tag{16} \]
\[ J_3 = \sum_{\langle i\sigma\rangle, \langle j\sigma'\rangle, \langle k\sigma''\rangle} u_{3}^{\sigma\sigma\sigma'}(x_{ij}) u_{3}^{\sigma'\sigma''}(x_{jk}), \tag{17} \]
where \( x_{ij} \) is the interparticle distance. Since the finite system with screened interactions is dominated by short-range correlations, we chose \( u_n(x) \) to have a simple Gaussian form
\[ u_{n}^{\sigma\sigma'}(x) = \delta_{n}^{\sigma\sigma'} \exp \left( -x^2/\gamma_{n}^{\sigma\sigma'} \right), \tag{18} \]
with \( \delta_{n}^{\sigma\sigma'} \) and \( \gamma_{n}^{\sigma\sigma'} \) variational parameters. Energy minimization improves the quality of the variational wave function and stabilizes the forward walking estimate of the expectation values on the DMC projected state.

Again the static structure factor is determined for different densities of electrons in the upper wire. In contrast to the calculations for the homogeneous system, the density of the electrons is not a direct input to the calculation. Instead, we control the number of electrons in the wire which are then free to relax according to the expectation values on the DMC projected state.

FIG. 10: (Color online) Static structure factor for a wire as in Fig. 9 but with finite length \( S(k) \) is plotted for 20, 40, 60, 70, 80, 90 and 100 electrons. The corresponding effective densities \( \tilde{r}_n \) are reported in the legend.

FIG. 11: (Color online) Density profile for electrons in the finite wire as in Fig. 10 plotted for half of the wire length. \( N = 20, 40, 60, 70, 80, 90 \) and 100 are considered.

In addition to the formation of a broad peak in the \( S(k) \) at \( 4k_F \) around \( N = 80 \), which corresponds to \( \tilde{r}_n = 2.3 \), the density profile \( n(x) = \langle \sum_i \delta(x-x_i) \rangle \) of the electrons also shows a clear cut off of the transition. At low densities, the electrons are distributed in order to minimize the interparticle repulsion. This leads to \( N \) oscillations in the density profile of the wire, a configuration also called "Wigner molecule" which corresponds to the \( 4k_F \) peak in the \( S(k) \). When the density is increased, the number of peaks in the density profile is reduced by a factor of two, the Pauli exclusion principle between like spin particles being the only factor that prevents the electrons from crossing each other. At the same time the \( 4k_F \) peak in the \( S(k) \) disappears and only a \( 2k_F \) singularity is present. The density is plotted in Fig. 11 for half of the wire as the system is symmetric under inversion around its center. This plot also suggests a transition near \( N = 80 \).

Surprisingly, the calculations with the confinement potential and the infinite wire give very similar structure factors in the vicinity of the transition, suggesting that the interparticle correlations are not strongly affected by the external confinement at those densities. At lower densities the peak at \( 4k_F \) is much larger for the homogeneous system because of the limited number of particles in the finite wire. Both the infinite and finite wires show a transition from a system with \( 2k_F \) correlations to a state where correlations have a \( 2r_s \) periodicity. The crossover occurs around \( r_s = 2.3 \), which corresponds to the density of \( 22 \mu m^{-1} \) in a GaAs heterostructure. This is very close to the density found by Steinberg et al. (20) \( \mu m^{-1} \) for the localization transition in wires where one subband is occupied. However it seems that in the experiment
the localization involves only few particles (up to 12 in the highest density localized state), i.e. only a section of the wire takes part in the transition. This is an important difference with respect to our calculations where the transition takes place throughout the system in a quite homogeneous way. A non homogeneous behavior is found at the edge of the wire where the confining potential in Eq. 14 turns upward. There the transition happens at higher densities, as one can see in Fig. 11. This can be understood in terms of a local mean field description. At the edge of the wire the effective chemical potential \( \mu_0 - V(x) \) is smaller, corresponding locally to a fluid at much lower density.

Apart from these features, we did not find any Wigner correlated patch embedded in a liquid-like system, which seems to be the experimental outcome. Therefore a more detailed analysis of the experimental setup is required to understand better the experiment. For instance, one of the top metallic gates used to tune the upper wire density could induce a plateau in the external potential, nucleating a Wigner region as suggested by Mueller. On the other hand, the role of disorder is not clear. Although in the liquid phase the system is in a ballistic regime, when the conductance is quantized the disorder could take over in the localized phase and affect the charge distribution in the wire. AlAs wires, where the disorder is stronger, revealed conductance resonances explained in terms of Coulomb blockade (CB) physics. CB behavior has also been found in the localized phase of GaAs wires.

Even if there are features that still need explanation, our calculations show that the electronic correlation plays a very important role at the experimental conditions, as the 2\( k_F \)-to-4\( k_F \) correlations transition takes place exactly in the proximity of the critical density for localization found in the experiment. In addition to this result, which is the main outcome of the paper, we also determined the charge and spin velocities by means of the QMC method explained in Sec. II and the effective WKB approximation, whereas the black triangles are determined using the QMC method described in Section II

The two lines are estimates due to the perturbative generalized random phase approximation (GRPA) \( v_F/\sigma_{GRPA} = 1/\sqrt{1 - V(2k_F)/(\pi v_F)} \). The green line for the gated wire (with \( R = 50 \)) uses the potential described by Auslaender et al whereas the dotted blue line uses the potential (Eq. 12) screened by the lower wire.

Last but not least, our WKB estimate of \( J \) turns out to be of the order of the experimental temperature \( (T = 0.25K) \) around \( n = 10\mu m^{-1} \). This means that at least the first few Coulomb blockade peaks in the experiment should be in a spin incoherent regime, where the LL description by Fiete et al. applies, although in the vicinity of the transition the spin degrees of freedom are not dominated by thermal broadening.

V. CONCLUSIONS

We have presented extensive quantum Monte Carlo calculations to study the properties of electrons constrained to one dimension with a harmonic confinement and interacting via several different potentials.

For unscreened interactions with a long range 1/\( x \) tail there are three different regimes. At high density the electrons behave as a correlated liquid, transitioning to a quasi Wigner crystal as the density decreases, whereas strong 4\( k_F \) correlations follow the LL predictions. We accurately determined the crossover density for various thicknesses and found that the crossover is pushed to higher densities for thinner wires. Finally at very low densities the charge degrees of freedom are described by spinless fermions and the spins decouple with exponen-
tially small exchange interactions. We approached this limit by using the WKB approximation.

When screening is introduced, the interactions are not long-range, and the quasi Wigner crystal order is destroyed. However, $4k_F$ correlations are still present even in the case of screened interactions. The spinless fermion regime acquires a new behavior when the wire is very thin and the screening makes the potential short-range. In this case the particles act as though they were non-interacting and spinless in analogy to physics previously studied for bosons with an infinite contact repulsion.

We applied our numerical approach to analyze a model chosen to realistically describe the double wire system studied in the experiments of Steinberg et al., where a localization transition is observed. Our model assumes screening due to a second wire described within linear response theory, and includes the finite length of the wire via the external potential derived in Ref. 8. We show that a crossover from a liquid to a state with $4k_F$ correlations occurs around the localization density found in the experiment. Additionally, our exact Monte Carlo calculations yield charge and spin velocities for this model in agreement with those observed in the experiment close to the transition. We stress that the observables such as the transition density and the spin velocity are particularly sensitive to the microscopic details of the model interaction. To reproduce all features of the experiment it may be necessary to include further refinements such as a more accurate modulation of the external potential due to the gates, the effects of higher subbands in the transverse direction and the full treatment of interwire electronic correlation by explicitly including the electrons in the other wire. However, the simple model considered here shows that the exact treatment of electronic correlation is essential to quantitatively describe the localization transition seen in experiments.

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