Charge and spin correlations of a one dimensional electron gas on the continuum

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We present a variational Monte Carlo study of a model one dimensional electron gas on the continuum, with long-range interaction (1/r decay). At low density the reduced dimensionality brings about pseudonodes of the many-body wavefunction, yielding non-ergodic behavior of naive Monte Carlo sampling, which affects the evaluation of pair correlations and the related structure factors. The problem is however easily solved and we are able to carefully analyze the structure factors obtained from an optimal trial function, finding good agreement with the exact predictions for a Luttinger-like hamiltonian with an interaction similar to the one used in the present study.

I. INTRODUCTION

Electrons in low dimensions, as found in modern semiconductor devices, are greatly affected by correlation effects that may dramatically change their behavior and bring about new phenomena and phases. Technological advances have reached the point where it is now possible to fabricate high mobility systems in which the electrons move essentially free and are intentionally confined at the nanoscale in suitable geometries. Though the details of the devices still play a role at the quantitative level, to a good approximation some of these systems provide a very close realization of simple electron gas models. We should emphasize that this is true only in low dimension and the experimental realization of a clean 3-dimensional (3D) electron gas (EG) in the quantum regime is in fact still out of sight, as is the long sought 3D Wigner crystal. Here, we focus our attention on a simple 1D model with long-range interaction, i.e., a quantum wire, with the aim of examining its structural properties.

A large variety of models have been proposed over the years for quantum wires. One may roughly distinguish two classes of systems, depending whether the wire is obtained from the confinement of a 3D or of a 2D or electron gas; or one may focus on the nature of the confinement, which can be harmonic, hard-wall like or Coulombic. In all these cases, the effective electron-electron interaction in the lowest subband of the transverse motion turns out to have a 1/r long-range tail, whereas the details of the confinement only affect the behavior at short range, which displays anyhow a divergence milder than 1/r, if any. Thus, if the interest is in the effect of the long range tail of the interaction, one may well resort to ad-hoc choices of the interaction or even to tight-binding models yielding Hubbard-like Hamiltonians with long range intersite interaction; however, this last choice may introduce processes (such as the Umklapp scattering) not present in continuum models. One should also recall that, for interacting Fermions in 1D, the familiar Fermi-liquid paradigm must be abandoned in favor of the Tomonaga-Luttinger liquid concept.

The above model wires have been studied at T = 0 employing several techniques ranging from DFT treatments to dielectric-formalism approaches of the STLS type, from exact diagonalization to density matrix renormalization group techniques, to bosonization techniques-the last approach being able to provide exact results for some properties if a linearized kinetic energy dispersion is assumed. Investigations of the homogeneous 1DEG on the continuum, performed with either the variational (VMC) or the diffusion Monte Carlo (DMC), are also available. Contrary to STLS predictions for the same model, DMC simulations yield no Bloch instability (spontaneous magnetization of the system), in accordance with the Lieb and Mattis theorem. They predict pair correlations that are consistent with a quasi Wigner crystal (strong charge correlations resulting in a divergent peak in the charge structure factor at 4k_F). However, they also appear to imply the presence of quasi antiferromagnetic order, i.e., a divergence of the spin structure factor at 2k_F in the unpolarized state, a result at variance with the findings of the bosonization technique. Rather than to the differences between models, such a discrepancy is likely to be due to the ergodicity problems encountered in both DMC and VMC simulations at strong coupling, as exchange between opposite spin electron is frozen out by the strong Coulomb repulsion. While in the DMC method a solution of this problem is not straightforward, in VMC simulations one may devise fairly simple ways of restoring ergodicity, thus establishing the true nature of spin correlations, as we show below.

II. MODEL AND WAVEFUNCTION

The Hamiltonian of our model quantum wire is, in units in which a_0^2 = \hbar^2\epsilon/(m^*e^2) = 1 and e^2/(2\epsilon a_0^2) = 1,

\[ H = -\sum_{i=1}^{N} \nabla_i^2 + 2 \sum_{i<j} V_6(|x_i - x_j|), \]  \tag{1}

\[ V_6(x) = (\sqrt{\pi}/2b)\exp\left(x^2/4b^2\right)\text{erfc}\left(|x|/2b\right), \]  \tag{2}

\]
with b a measure of the wire width. Above, ϵ is the dielectric constant of the semiconductor and m* the effective mass of the carriers. The pair interaction \( V_\parallel(x) \), which is finite at the origin, \( V_\parallel(0) = \sqrt{\pi}/(2b) \) and decays as \( 1/x \) for \( x \gg b \), is obtained from an harmonic confinement of the 3DEG, after projection on the lowest subband of transverse motion\(^\text{[2]}\); it thus provides a good approximation to the 3D system at low density \( \rho \), i.e., \( r_s = 1/2\rho \gg \pi b/4 \), with the density parameter \( r_s \) also providing an estimate of the Coulomb coupling, as ratio between average potential and kinetic energies.

We use VMC simulations and focus on the ground state properties of a thin wire (\( b = 0.1 \)) on a fairly wide coupling range (\( 1 < r_s < 10 \)), thus considering only unpolarized states\(^\text{[13, 17]}\). To this end, we resort to a Slater-Jastrow wavefunction\(^\text{[18]}\) \( \Psi_T = JD^\dagger D \), with \( D^\sigma \) a determinant of \( N^\sigma \) plane waves and \( J = \exp[-\sum_{i<j} u(|x_i - x_j|)] \), with \( u(x) \) a two-body pseudopotential to be optimized. This is the simplest correlated wavefunction for an unpolarized Fermion state with homogeneous density and can be further improved with the inclusion in the Jastrow factor \( J \) of higher order pseudopotentials\(^\text{[12]}\). Our goal here is a careful finite-size scaling extrapolation of structural properties, to obtain the long-range behavior of pair correlation functions. Thus, to reduce the finite size bias we keep \( N^\uparrow = N^\downarrow \) odd, in order to avoid shell degeneracy effects, use periodic boundary conditions and Ewald-sum\(^\text{[14, 16, 18]}\) the pair potential \( V_\parallel(x) \).

We remind the reader that in 1D the nodes of the Fermionic ground state (of given symmetry) are know exactly\(^\text{[20]}\), as they are fully determined by exchange (antisymmetry, and coincide in particular with those of the above wavefunction for the unpolarized state. Thus, DMC provides in principle exact energies\(^\text{[14, 16, 18]}\) that may serve as benchmark for the VMC simulations when optimizing the Jastrow factor \( J \). As starting point for our simulations we take a two-body pseudopotential of the RPA type\(^\text{[13, 21]}\), which in Fourier space reads

\[
2\rho\tilde{u}_{RPA}(k) = -S_0(k)^{-1} + \sqrt{S_0(k)^{-2} + 4\rho\tilde{V}_b(k)/k^2},
\]

with \( S_0(k) = (k/2k_F)^2(2k_F-k)^2(k-2k_F) \) the structure factor of a non interacting 1DEG,

\[
\tilde{V}_b(G) = E_1(b^2G^2) \exp(b^2G^2)
\]

the Fourier transform of the interaction, and \( \theta(x) \) and \( E_1(x) \) respectively the Heaviside and the exponential integral functions.

The repulsive nature of the pair interaction \( V_\parallel(x) \) is directly reflected in the pseudopotential, which is shown in Fig. 1. The pseudopotential is repulsive and the repulsion increases appreciably with decreasing the density (increasing the \( r_s \)). Thus, as the density is lowered electrons are kept apart more and more effectively and this results in a quasi long range order which can be described as a quasi Wigner Crystal\(^\text{[13]}\). Though the pseudopotential remains finite at contact, the Jastrow factor becomes exponentially small yielding what may be seen as pseudonodes of the wavefunction. These pseudonodes have no particular effect on like spin electrons, as the wavefunction is already vanishing at contact for such electrons and most importantly particle exchanges are explicitly summed over in the determinants. On the contrary, the effect on opposite spin electrons when combined with the reduced dimensionality may become dramatic. In a random walk in configuration space with importance sampling given by the Slater-Jastrow wavefunction, the RPA pseudopotential tends to freeze out the exchange between opposite spin electrons and may cause ergodicity problems, which show up in spin correlations\(^\text{[14, 16]}\).

Evidently, it is not only the presence of the pseudonodes to cause problems but also the slope with which the pseudonodes are approached, on the scale of the interparticle distance. When such a slope becomes sufficiently large, naive algorithm may become inefficient in sampling inequivalent pockets in configuration space, delimited by the pseudonodes.

**III. ERGODICITY AND VMC OPTIMIZATION**

Ergodicity becomes an issue in the present context because in 1D there is no exchange without crossing, for opposite spin electrons. With increasing the coupling, the maximum displacement \( \delta \) has to be made smaller (on the \( r_s \) scale), to keep the acceptance high, and this reduces the exchange frequency \( \nu = \) spin flips/total moves substantially. The problem is very serious in DMC simulations, as very small displacements are necessary\(^\text{[22]}\), to keep the time step error small, and a direct sampling of spin exchange is not straightforward. On the contrary, in the VMC method it is relatively easy to devise effective ways of keeping \( \nu \) above a suitable threshold (\( \approx 0.01 \)) ensuring ergodicity. The simplest choice is to work at acceptance appreciably lower than 50%, i.e., at larger \( \delta \).
TABLE I: Exchange frequency \( \nu \) at \( r_s = 10 \) and \( N = 22 \). \( \delta \), \( \alpha \) and \( E \) are the maximum displacement of the MC move, the average acceptance, and the energy per particle. In all cases an optimized (scaled) RPA pseudopotential (see text) is used.

| Sampling | \( \delta/2r_s \) | \( \alpha \) | \( \nu \) | \( E \) |
|----------|------------------|---------|-------|-------|
| \( \Psi_T \) | 1.3 | 0.49 | 6.06 \cdot 10^{-1} | -0.474825(9) |
| \( \Psi_T \) | 3.0 | 0.24 | 1.03 \cdot 10^{-2} | -0.474827(9) |
| \( \Psi_G \) | 1.3 | 0.51 | 7.36 \cdot 10^{-3} | -0.474832(8) |

Other possible choices involve either umbrella sampling / reweighting, i.e. the use of configurations generated from a guidance function \( \Psi_G \) less repulsive than the trial function \( \Psi_T \) considered above, or the use of a generalized Monte Carlo move, involving the direct sampling of exchange between opposite spin electrons. One may also consider combinations of the above. In Tab. II we focus our attention on the first two choices, for the worst case examined here, i.e., \( r_s = 10 \). It is clear that both the large \( \delta \) and the \( \Psi_G \) recipes are effective in keeping \( \nu \) close to value \( \approx 0.01 \) found at small couplings, \( r_s \approx 1 \), where there are no apparent signals of nonergodicity. Indeed we find that keeping \( \nu \approx 0.01 \) the noisy patterns previously found in the spin structure factor disappear. On the other hand, the energy does not seem to depend on \( \nu \) and this is likely due to the fact that at strong coupling different spin configurations are almost degenerate. In the following we restrict our attention to the large \( \delta \) prescription which has the advantage of maximum simplicity.

To get an accurate description of correlation functions we systematically optimize \( \Psi_T \), employing the variance minimization method. As the plane-wave determinants provide the exact nodes for our 1D system, we only need to optimize the Jastrow factor \( J \), i.e., the two-body pseudopotential \( u(x) \), for which we have considered both a scaled RPA form \( u_a(x) = \alpha u_{RPA}(x) \) and a systematic expansions in terms of Chebyshev polynomials

\[
u(x) = \sum_{m=1}^{m_{max}} a_m T_{2m}(2|x|/L - 1), \tag{5}
\]

satisfying the continuity of the first derivative at the edge of the simulation box, \( u'(L/2) = 0 \). The results of the optimization are summarized in Tab. II in terms of the correlation energy \( E_c = E_0 - E_{HF} \), with \( E_0 \) and \( E_{HF} \) the exact (DMC) and Hartree-Fock energies. We find that the scaled RPA form is essentially equivalent to the true two-body pseudopotential, obtained with about 10 terms in the sum of Eq. 5. Moreover, adding a three-body term in \( J \), within a factorization ansatz à la Feynman retaining the first two \( l \)-components does not improve our results in any appreciable manner. Therefore in the following we use a scaled RPA psudopotential optimized for each \( N \).

FIG. 2: Peak in the charge structure factor versus the system size. The curves are fits to the VMC predictions (symbols).

IV. PAIR CORRELATIONS

According to the predictions of the bosonization technique applied to a Luttinger Hamiltonian (linearized kinetic energy) with long-range interaction, charge correlations exhibit long range tails resulting in a divergent peak at \( 4k_F \) in the charge structure factor \( S_{++}(k) = \langle \rho_+(k)\rho_+(-k) \rangle/N \), whereas spin correlations decay faster and a finite peak is found at \( 2k_F \) in the spin structure factor \( S_{--}(k) = \langle \rho_-(k)\rho_-(k) \rangle/N \). Here, \( \rho_\pm(k) = \rho_{1}(k) \pm \rho_{2}(k) \) is the Fourier component of the charge (spin) density. We have performed VMC simulations for \( b = 0.1 \), \( r_s = 1, 2, 6, 10 \), \( N = 10, 22, 42, 82, 162 \), and computed the above structure factors at several \( k \) values. In Fig. 2 and 3 we give the peak heights \( N(4k_F) = S_{++}(4k_F, N) \) and \( S(2k_F) = S_{--}(2k_F, N) \), which appear to be increasing functions of \( N \). As such heights are determined by the long-range behavior of correlations we expect them to scale with \( N \) similarly to what found for the long-range Luttinger liquid of 8, for which at large \( N \) one readily obtains

\[egin{align*}
S(2k_F) &= a_3(\sqrt{\log L} + 1/c) \exp(-c\sqrt{\log L}) + a_4, \\
N(4k_F) &= a_1 L \exp(-4c\sqrt{\log L}) + a_2,
\end{align*}
\tag{6}
\]

with \( L = 2r_sN \) and \( c, a_1,a_2,a_3,a_4 \) model and density dependent. We have used Eqs. 4 to fit our results, obtaining first \( a_1, a_2, c \) from the fit of \( N(4k_F) \) and then \( a_3, a_4 \).

TABLE II: Total energy \( E_{tot} \), correlation energy \( E_c \), and percentage of correlation energy \( \%E_c \) for \( b = 0.1 \), \( r_s = 10 \), and \( N = 22 \). The fraction of the correlation energy recovered is computed from DMC calculations which provide the exact GS energy for a 1DEG.

|          | \( E_{tot} \)     | \( E_c \)     | \%\( E_c \)     |
|----------|------------------|---------|-------|
| RPA      | -0.47207(2)      | -0.20519(56) | 0.9830(15) |
| Scaled RPA | -0.474825(9)     | -0.20794(55) | 0.9962(15) |
| Chebyshev| -0.474900(9)     | -0.20802(55) | 0.9965(15) |
FIG. 3: Peak in the spin structure factor versus the system size. The curves are fits to the VMC predictions (symbols).

![Graph](image)

**TABLE III:** Fit of the peak of the charge and spin structure factors: reduced $\chi^2$ and interaction (fit) parameter $c$.

| $r_N$ | $\chi^2_1$ | $\chi^2_2$ | $c$ |
|-------|------------|------------|-----|
| 1     | 4.1        | 3.5        | 0.71 |
| 2     | 4.7        | 1.5        | 0.78 |
| 6     | 0.55       | 0.03       | 0.80 |
| 10    | 3.6        | 1.3        | 0.88 |

from the fit of $S(2k_F)$, with $c$ fixed by the fit of $N(4k_F)$. As it can be seen from Fig. 2, 3 and Tab. III the long-range tails implied by Eqs. 6 are indeed consistent with our VMC results, yielding a finite $S(2k_F)$ in the thermodynamic limit. We have reason to believe that a further improvement of the $\chi^2$ would be obtained by discarding the smaller values of $N$ in favor of larger ones, on the ground that Eqs. 6 only embody the long-range behavior of correlations.

**V. SUMMARY**

In conclusion, we have shown that a relatively simple (unbiased) optimization of the wavefunction is able to yield correlations functions for a 1DEG on the continuum which are in qualitative agreement with the exact predictions of Schulz 8 for a Luttinger Hamiltonian with long-range interactions. The correlations that we find do support the existence of a quasi Wigner crystal and a non-ordered unpolarized magnetic phase. These results are at variance with what previously found for the same model wire with VMC[14, 15] and DMC[14] simulations, as those calculations were biased by non-ergodicity. The results found here are strongly corroborated by very recent simulations[25] with a novel lattice regularized DMC (LRDMC) method[26], which significantly alleviates the lack of ergodicity in the standard DMC. In particular, we find[23] that the time projection implemented by the LRDMC only produces minor quantitative changes in the charge and spin peak heights, leaving our present conclusions unchanged.

[1] Nanostructure Physics and Fabrication, ed. by M. Reed and W.P. Kirk (Academic Press, Boston, 1989); C. Weisbuch and B. Vinter, Quantum Semiconductor Structures, (Academic Press, Boston 1991).

[2] See, e.g., S. De Palo, M. Botti, S. Moroni, and G. Senatore, cond-mat/0410145 and to be published.

[3] W. I. Friesen and B. Bergesen, J. Phys. C 13, 6627 (1980).

[4] A. Gold and A. Ghazali, Phys. Rev. B 41, 7626 (1990).

[5] G. Y. Hu and R. F. O’Connel, Phys. Rev. B 42, 1290 (1990).

[6] G. Y. Hu and S. Das Sarma, Phys. Rev. B 48, 5469 (1993).

[7] Y. Sun and G. Kirchenow, Phys. Rev. B 47, 4413 (1993).

[8] H. J. Schulz, Phys. Rev. Lett. 71, 1864 (1993).

[9] G. Fano and F. Orlolini, A. Parola, L. Ziosi, Phys. Rev. B 60, 15654 (1999).

[10] S. Capponi and D. Poilblanc, T. Giamarchi, Phys. Rev. B 61, 13410 (2000).

[11] K. Schonammer and V. Meden, Am J. Phys. 64, 1168 (1996); J. Voit, Rep. Prog. Phys. 58 977 (1995).

[12] L. Camels and A. Gold, Europhys. Lett. 39, 539 (1997).

[13] D. Poilblanc, S. Yunoki, S. Maekawa, and E. Dagotto, Phys. Rev. B 56 R1645 (1997).

[14] A. Malatesta, Ph.D. Thesis (in english), University of Trieste (1999); it can be obtained from senatore@ts.infn.it.

[15] A. Malatesta and G. Senatore, J. Phys. IV 10, Pr5-341 (2000).

[16] M. Casula, Laurea Thesis (in italian), University of Trieste (2001); it can be obtained from senatore@ts.infn.it.

[17] E. Lieb and D. Mattis, Phys. Rev. 125, 164 (1962).

[18] See, e.g., D. Ceperley, Phys. Rev. B 18, 3126 (1978).

[19] See, e.g., S. Moroni, S. Fantoni, and G. Senatore, Phys. Rev. B 52, 13547 (1995).

[20] D. M. Ceperley, J. Stat. Phys. 63, 1237 (1991).

[21] T. Gaskell, Proc. Phys. Soc. 77, 1182 (1961), ibidem 80, 1091 (1962).

[22] P. J. Reynolds and D. M. Ceperley, B. J. Alder, W. A. Lester, Jr., J. Chem. Phys. 77, 5593 (1982).

[23] D.M. Ceperley and M. Kalos, in Monte Carlo Methods in Statistical Physics ed. K. Binder (Springer, New York, 1979).

[24] C. J. Umrigar, K. G. Wilson, J. W. Wilkins, Phys. Rev. Lett. 60, 1719 (1988).

[25] M. Casula, S. Sorella, and G. Senatore, to be published.

[26] M. Casula, C. Filippi, and S. Sorella, cond-mat/0502388 and to be published.