Unscreened Coulomb repulsion in the one dimensional electron gas

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A tight binding model of electrons interacting via bare Coulomb repulsion is numerically investigated by use of the Density Matrix Renormalization Group method which we prove applicable also to very long range potentials. From the analysis of the elementary excitations, of the spin and charge correlation functions and of the momentum distribution, a picture consistent with the formation of a one dimensional “Wigner crystal” emerges, in quantitative agreement with a previous bosonization study. At finite doping, Umklapp scattering is shown to be ineffective in the presence of long range forces.

One dimensional electron models are often used to interpret the behavior of strongly anisotropic physical systems in condensed matter, like organic conductors, charge transfer salts and certain semiconductor nanostructures. These systems can be modeled in terms of a tight binding hamiltonian with effective electron repulsion, which can be either short or long ranged, depending on the extent of interchain screening. The prototype of the short range models is the exactly solvable one dimensional repulsive Hubbard model which is known to be in the universality class of Luttinger liquids, showing metallic properties and antiferromagnetic spin correlations at every finite doping. However, this picture may dramatically change if screening is not effective in reducing the range of the bare Coulomb potential. This possibility is well known in quantum chemistry where the Pariser-Parr-Pople model (PPP), describing conjugated polyenes, has exactly the same structure of a tight binding model with unscreened Coulomb-like interaction. This Hamiltonian has been studied in small lattices by variational methods, like unconstrained Hartree-Fock, suggesting the development of a charge density wave (CDW) leading to an antiferromagnetic insulating ground state in the thermodynamic limit. Exact diagonalizations, recently performed in systems with few electrons, instead provide evidence in favor of a metallic behavior. Unfortunately, finite size effects inhibited the study of correlation functions leaving open the two possibilities of a Luttinger liquid or of a CDW metal where the charge carriers can be identified as sliding density waves, while electron-like quasiparticles are absent. The latter scenario was in fact proposed by Schulz in a seminal bosonization study. Here, the picture of a one dimensional Wigner crystal emerged, characterized by extremely long range tails for the charge correlation functions at the density dependent wavevector $4k_F$, together with weaker antiferromagnetic correlations at $2k_F$.

In order to clarify the physics of one dimensional systems with unscreened Coulomb repulsion, we performed a Density Matrix Renormalization Group (DMRG) study for the PPP model. Results for the excitation spectrum in the spin and charge channels are presented. The density and magnetic structure factors have been computed both at half filling and in the doped system. A physical insight on the nature of charge carriers has been obtained through the study of the momentum distribution of the electrons.

DMRG is an extremely accurate numerical method, especially devised for one dimensional problems, which can easily handle system sizes two or three times larger than usual diagonalization algorithms, thereby drastically reducing finite size effects. DMRG gives the exact spectrum of the hamiltonian in a reduced Hilbert space and therefore it provides a variational bound to the exact ground state energy. The method also allows for a self consistent evaluation of the errors introduced by truncation, by checking the unitarity sum rule satisfied by the exact density matrix, which reflects the completeness of the Hilbert space.

The model we have studied is defined by $N$ electrons on a $L$ site ring with hamiltonian

$$
H = -t \sum_{i,\sigma} \left( c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c. \right) + \frac{U}{2} \sum_{i,j} \frac{(n_i - \bar{n})(n_j - \bar{n})}{1 + \gamma_0 d_{ij}}
$$

(1)

where $c_{i,\sigma}$ is a fermionic annihilation operator, $n_i = \sum_\sigma c_{i,\sigma}^\dagger c_{i,\sigma}$ is the density operator at site $i$ with average value $\bar{n} = N/L$ and $d_{ij}$ is the chord distance on the circle:

$$
d_{ij} = \frac{|\sin(i - j)\frac{2\pi}{L}|}{\sin\frac{\pi}{L}}
$$

(2)

The parameter $\gamma_0$, which controls the strength of the long range Coulomb repulsion, is fixed at $\gamma_0 = 0.053907$, following the Mataga-Nishimoto prescription. Here we present extensive results for a representative value interaction strength $U/t = 13.55$.

The physics underlying the half filled case (i.e. $\bar{n} = 1$) is well established. In the strong coupling limit (i.e. $U \rightarrow \infty$), charges are frozen and the low energy configurations just correspond to different spin orientations: in a bipartite lattice, the ground state is always a non
degenerate spin singlet and it is expected to show correlations typical of one dimensional antiferromagnets: $< \mathbf{S}_n \cdot \mathbf{S}_m > \sim (1)^n/n$, like in the Heisenberg model. Spin excitations are gapless with linear dispersion relation. Analogously to the Hubbard model, for every strength of the Coulomb repulsion, a charge gap develops, a gap in the spin excitation spectrum, as a precursor to charge ordering with different periodicity, i.e. the one dimensional analog of a "stripe" phase, or the formation of a gap in the spin excitation spectrum, as a precursor to phase separation, which is inhibited by long range forces.

In order to understand which picture correctly describes the physics of correlated electron systems with long range interactions, we numerically studied the PPP model \cite{3} at the two electron densities $\bar{n} = 1/2$ and $\bar{n} = 3/4$ corresponding to $k_F = \pi/4$ and $k_F = 3\pi/8$ respectively. These choices of filling factors are suggested by the necessity to perform accurate size scaling keeping, at the same time, a limited number of degrees of freedom. Calculations have been performed in lattices up to $L = 80$ sites and total number of electrons up to $N = 60$. The chosen electron densities are represented by small fractions, hence we expect that commensurability effects may be enhanced for these cases: If the model is prone to a CDW instability, the systems studied in this work should clearly suggest the tendency toward charge ordering. Our DMRG code is written in such a way to cope with long range potentials. The dimension of the reduced Hilbert space is always larger than $10^6$, the truncation error is at most $10^{-5}$ and the correlation functions are translationally invariant up to a relative error of $2 \times 10^{-2}$. Further details on the algorithm can be found in Ref\cite{3}.

As a first step, we calculated the charge spectrum, i.e. the ground state energies $E(N+1)$ and $E(N-1)$ obtained by adding and removing one electron to the reference state with $N = \bar{n}L$ particles. In order to have a non-degenerate singlet ground state, we imposed periodic or anti-periodic boundary conditions thereby realizing the closed shell condition in the non-interacting limit on the reference state. The finite size gap is defined as the difference between the upper and lower estimate of the chemical potential:

$$\Delta_\rho = \mu_+ - \mu_- = \frac{1}{2} [E(N+1) + E(N-1) - 2E(N)]$$

Although $\Delta_\rho$ does not coincide with the true charge gap we can infer that the charge gap is zero if $\Delta_\rho$ vanishes in the thermodynamic limit. Conversely, the spin gap $\Delta_\sigma$ is just the energy difference between the singlet and the triplet spin sectors at fixed number of particles. The finite size scaling of our results, shown in Fig. 1, clearly indicates the gapless nature of the excitation spectrum, ruling out the possibility of charge ordering in the ground state and confirming the irrelevance of Coulomb repulsion on the structure of spin excitations in agreement with previous diagonalization data. The analysis of correlation functions provides a deeper information on the physical nature of the ground state. In particular, we studied the charge and spin structure factors defined by:

$$R(q) = \frac{1}{L} \sum_{l,m} e^{iq(l-m)} < n_l - \bar{n} > (n_m - \bar{n}) >$$

$$S(q) = \frac{1}{L} \sum_{l,m} e^{iq(l-m)} < S_l^z S_m^z >$$

The Fourier transform $R(q)$ of the equal time density-density correlation function shown in Fig. 2 displays a remarkable collapse of data relative to different sizes, with the single exception of the peak region at $q = 4k_F$. The peak value, plotted as a function of $L$ in Fig. 3, is well fitted by the expected form $R(4k_F) \sim L \exp(-4c\sqrt{\ln L})$ deduced from the bosonization analysis \cite{3} suggesting that
quasi long range order develops in the system. Notice the appreciable curvature of the data which reflects the presence of the exponential term in the fitting formula and, in turn, indicates a very slow decay of density correlations in real space. The holes effectively repel each other and stay almost rigidly at the maximum attainable average distance $\lambda = 1/\bar{n}$ but, as expected, hole correlations vanish at large distance, in agreement with Eq. (3). A much weaker singularity seems to be present at wavevector $2k_F$, but the data do not allow for a systematic analysis of this further feature, also predicted by the bosonization analysis of Ref. 4. Other interesting information can be extracted from the small $q$ behavior of $R(q)$ which is related to the low energy excitation spectrum. According to the bosonization formulas, the structure factor should behave as $R(q) \sim q |\ln q|^{-1/2}$. This form well represents the DMRG data, as shown in Fig. 4. Note that such an expression is quite specific to the bare Coulomb interaction and differs from the usual Luttinger liquid results, where $R(q) \sim K_q (q/\pi)$. A similar analysis can be carried out for the magnetic properties of the model. In Fig. 5 the magnetic structure factors $S(q)$ corresponding to the previously discussed choices of parameters are shown. The collapse of points on the same smooth curve should be again appreciated. The dominant peak occurs at $q = 2k_F$, as expected, and its height, reported in Fig. 6, scales as $a_0 - a_1 (\sqrt{\ln L} + 1/c) \exp(-c \sqrt{\ln L})$ in agreement with the bosonization prediction (3). Here $a_0$ and $a_1$ are fitting parameters, while the constant $c$ is fixed to the same value obtained from the fit of the density structure factor shown in Fig. 3. Contrary to the results obtained for $R(q)$, the small $q$ behavior of $S(q)$ is accurately given by the linear relation $S(q) \sim (q/4\pi)$ corresponding to $K_q = 1$, as expected for all the gapless, $SU(2)$ invariant, one dimensional electron systems.

The previously discussed properties of the PPP model, emerging from the DMRG analysis, are consistent with the Wigner crystal model suggested by the bosonization study: away from half filling, the system is gapless both in the charge and spin sectors but, at the same time, it supports extremely long ranged density correlations. Following Ref. 3, we may consider two different pictures, consistent with the observed metallic properties of this model. The first one corresponds to a Luttinger liquid scenario, where the electrons have a sort of “Fermi surface” satisfying the Luttinger theorem. In this case, although the low energy excitations are always collective in one dimension, the charge carriers in the system may be still identified with dressed electrons. Instead, according to the second picture, the absence of a gap in the charge spectrum is due to the Wigner crystal nature of the ground state and to the long range decay of density correlations. The quasiparticles cannot be identified with electrons any more and consequently the electron momentum distribution is smooth at the Fermi momentum, with an extremely weak essential singularity, as reported in Eq. (3). DMRG data for the momentum distribution for given spin $n(q)$ are shown in Fig. 7, while a size scaling of the finite size jump at $q = k_F$ is plotted in Fig. 8. Again, the asymptotic scaling
\[ \Delta n(k_F) \sim \bar{L} e^{-c'(\ln \bar{L})^{3/2}} \] (6)
predicted on the basis of the bosonization result (3) gives a quite good representation of numerical data.

In conclusion, we have tried to clarify the physics underlying the presence of unscreened Coulomb interaction in one dimension. Accurate DMRG data are fully consistent with the picture of a Wigner crystal showing metallic properties, with slowly decaying density correlation and gapless charge and spin excitation spectra. At least in one dimension, this numerical investigation rules out other scenarios, like pinned CDW or even some precursor of off-diagonal long range order.

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FIG. 1. Charge gap $\Delta_\rho$ and spin gap $\Delta_\sigma$, in units of $t$, versus the inverse chain length $L$. The density is $\bar{n} = 3/4$.

FIG. 2. Fourier transform $R(q)$ of the equal time density-density correlation function. The density is $\bar{n} = 1/2$ in (a), $\bar{n} = 3/4$ in (b).

FIG. 3. Fit of $R(4k_f)$ with respect to the bosonization result. The circles are DMRG results for density $\bar{n} = 1/2$ and the solid line is a function of the form $aL \exp(-4c\sqrt{\ln L})$ with $a = 1.93$ and $c = 0.54$.

FIG. 4. Small momentum behavior of the charge structure factor. We plot $R(q)$ divided by the expected limiting form $q|\ln(q)|^{-1/2}$. The density is $\bar{n} = 3/4$. 
FIG. 5. Fourier transform $S(q)$ of the equal time spin-spin correlation function. The density is $\bar{n} = 1/2$ in (a) and $\bar{n} = 3/4$ in (b).

FIG. 6. Fit of $S(2k_f)$ with respect to the bosonization result. The circles are DMRG results for $\bar{n} = 1/2$ and the solid line is a function of the form $a_0 + a_1 (\sqrt{\ln L} + 1/c) \exp(-c\sqrt{\ln L})$ with $a_0 = 1.12$, $a_1 = 0.68$ and $c = 0.54$ (obtained from Fig. 3).

FIG. 7. Momentum distribution function for given spin $n(q)$. The density is $\bar{n} = 1/2$ in (a) and $\bar{n} = 3/4$ in (b).

FIG. 8. Fit of the finite size jump at $k_f$ of the momentum distribution with the expression: $\Delta n(k_f) = aL e^{-c' \ln(L)^{3/2}}$. The parameters are: $a = 0.493781$, $c' = 0.631772$ for $\bar{n} = 1/2$ (curve A) and $a = 0.491581$, $c' = 0.611964$ for $\bar{n} = 3/4$ (curve B).