Quantum Monte Carlo Study of electrons in low dimensions

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Abstract. We report on a diffusion Monte Carlo investigation of model electron systems in low dimensions, which should be relevant to the physics of systems obtainable nowadays in semiconductor heterostructures. In particular, we present results for a one dimensional electron gas, at selected values of the coupling strength and confinement parameter, briefly analyzing the pair correlations and relating them to predictions by Schulz for a Luttinger liquid with long–range interactions. We find no evidence of the the Bloch instability yielded by approximate treatments such as the STLS and DFT schemes.

1. INTRODUCTION

Electrons in low dimensions, as found in modern semiconductor devices[1], are greatly affected by correlations effects that may dramatically change their behavior and bring about new phenomena and phase transitions. However, at zero magnetic field and in simple systems, such as layers or wires, very low densities are necessary for correlations to play an important role. The situation is somewhat better in coupled systems. The additional correlations due to the interlayer (or interwire) interactions may help in pushing transitions to larger and more easily accessible densities[2], yielding richer phase diagrams and possibly new phenomena, such as superconductivity or excitonic condensation[3]. In all cases, the quantum Monte Carlo technique provides an effective tool, which allows the determination of the static properties of these systems with unprecedented accuracy[4, 5]. While in the invited paper delivered at the St-Malo by one of us (GS) results were presented for both an electron-hole bilayer and a model quantum wire, due to lack of space here we shall restrict to the latter system. A detailed account of the electron–hole bilayer simulations will be given elsewhere[6].

Perhaps, the theoretical interest for one-dimensional (1D) models is due in part to their inherent simplicity, which often results in exact solutions[7]. In fact, the problem of interacting Fermions simplifies in one dimension and one can show that the familiar concept of Fermi liquids has to be abandoned in favor of that of Tomonaga-Luttinger liquids[8]. The interest in 1D models has grown even bigger in recent years, thanks to the advances in fabrication techniques and the realization of the so called quantum wires[9, 10, 11], i.e., quasi-one-dimensional electron systems. Thus, the investigation of model 1D electron gases with numerical simulations, which yield results of high accuracy if not exact, is particularly appealing—both in relation to experiments and to other theoretical approaches.

2. THE MODEL

In a quantum wire the electronic motion is confined in two directions (say y and z) and free in the third one, x. In the simplest approximation, one assumes that the energy spacing of the one-particle orbitals
for the transverse motion is sufficiently large, so that only the orbital lowest in energy, say $\phi(y, z)$, needs to be considered. Hence the total wavefunction of the many-electron system will factorize in an irreducible many body term for the $x$ motion, $\Psi(x_1, \ldots, x_n)$, times a product of $\phi$’s, one per particle. Tracing out the transverse $(y,z)$ motion from the full Schrödinger equation yields an effective 1D problem with an effective 1D interparticle potential. Evidently, different models of confinement yield different effective potentials. One of the first models assumes a harmonic confinement in the transverse plane. More recently a hard wall confinement has been investigated, with the electrons moving freely in a cylinder of given radius. One may also start from the 2D electron gas and apply a confining potential in one direction; again, both harmonic and hard wall confinements have been considered.

Here, we choose the model of Ref. [11], with a harmonic confining potential $U_c(r) = (\hbar^2 / 8m^*b^4)(y^2 + z^2)$ and a coulombic electron-electron interaction $e^2 / \epsilon r$. The resulting effective 1D potential is readily shown to be $v(x) = (e^2 / \epsilon)(\sqrt{\pi} / 2b) \exp[(x/2b)^2] \text{erfc}[|x|/2b]$, with Fourier transform $v(q) = (e^2 / \epsilon)E_1[(bq)^2] \exp[(bq)^2]$. Above $m^*$ and $\epsilon$ are, respectively, the effective mass of the carriers and the dielectric constant of the medium in which the carriers move, and $b$ measures the wire width. One can easily check that $v(x)$ is long ranged, with a Coulomb tail $e^2 / \epsilon |x|$, and is finite at the origin, $v(0) = (e^2 / \epsilon b)(\sqrt{\pi} / 2)$. The 1D system is made neutral by introducing a background that cancels the $q = 0$ component of the pair interaction.

Earlier investigations of this model have employed the so-called STLS approximation, either in its original version or in its sum rule approach. Both the paramagnetic and the ferromagnetic phases have been studied and the occurrence of a Bloch instability [transition from the paramagnetic to ferromagnetic state] has been predicted. This, according to the authors, could explain the anomalous plateau which has been observed in the conductance of GaAs quantum wires, in the limit of single channel occupancy.

### 3. DMC RESULTS

To study our model quantum wire we resort here to fixed-node diffusion Monte Carlo (DMC) simulations. As the exact nodes are known in 1D, for a given number of particles we obtain exact estimates of the energy, within the statistical error—the small systematic time step error involved with the imaginary time integration was in fact extrapolated out. The estimates of other properties, such as static correlation functions and momentum distributions, remain approximate though very accurate. Below, we present some of our results for the energy and the structure, skipping completely the technical details of our calculations which can be found elsewhere.

We have performed simulations for three different values of the wire width, $b/a_B^\ast = 4, 1, 0.1$, at selected values of the coupling parameter $r_s$, defined in 1D by $\rho = N/L \equiv 1/2r_sa_B^\ast$. Here, $a_B^\ast = \hbar^2 \epsilon / m^*e^2$ is the effective Bohr radius of the material. We should remark that for the model at hand the coupling strength, defined as the ratio between the potential energy of a pair of particles at the mean distance $r_s a_B^\ast$ and the Fermi energy, is proportional to $r_s \times [r_s a_B^\ast v(r_s a_B^\ast)] = r_s \times f(r_s a_B^\ast/b)$, with $f(x)$ a growing function of $x$. Thus, at fixed $b$, the coupling actually increases more than linearly with $r_s$, whereas at given $r_s$ the coupling increases with decreasing $b$—reflecting the obvious fact that a narrower wire enhances the effect of the Coulomb repulsion.

### 3.1 The Energy

Our DMC ground state energies for wires with $b = 4a_B^\ast$ and $b = a_B^\ast$ are shown in Fig. together with the results of the STLS scheme, which is easily solved numerically. We should note here that the alternative sum rule approach to STLS yields results somewhat different from the present...
Figure 1: DMC ground state energy per particle, in $Ry^* = e^2/2e^*B$, of the paramagnetic (squares) and ferromagnetic (circles) fluids, in the thermodynamic limit $N = \infty$. The error bars are much smaller than the symbols. The predictions of STLS are given by the black and gray line, respectively for the paramagnetic and ferromagnetic phase. The insets show the Bloch instability yielded by the STLS scheme but not by our DMC simulations.

An additional comment, which is naturally prompted by Fig. 1, is that at intermediate and large coupling the STLS performs much better for the ferromagnetic phase than for the paramagnetic one. This is most easily appreciated by looking at the insets in the figure. In fact, one may argue on general grounds that it is easier to describe the fully spin polarized phase, as part of the correlation is automatically built in by the symmetry constraints.

3.2 The Structure

In a quantum wire interactions are enhanced, due to the reduced dimensionality, and strong ordering may thus arise at large coupling, even though genuine crystalline order is generally forbidden in 1D. In fact a 1D system with an interparticle potential decaying as $1/|x|$ is borderline, in this respect[23]. Ordering may be characterized in terms of structure factors, which measure ground state correlations between Fourier components of one body densities. Thus, we shall focus on the number and magnetization static structure factors, respectively $S_{nn}(k)$ and $S_{mn}(k)$, which are defined by $S_{\alpha\beta}(k) = \langle \rho_{\alpha}(k)\rho_{\beta}(-k) \rangle/N$, with the number density $\rho_n(k) = \rho_{\uparrow}(k) + \rho_{\downarrow}(k)$ and the magnetization...
Figure 2: Static structure factor of the paramagnetic fluid. The left panel gives extrapolated DMC estimates for 22 particles and $b = a_B^*$, at $r_s = 1, 2, 6, 10$; the errors are not visible on this scale. The right panel gives the predictions of STLS (dashed curves) and DSTLS (full curves). In all cases a decreasing slope at the origin corresponds to increasing $r_s$. Also, for the DSTLS only results for $r_s$ up to 6 are shown.

density $\rho_m(k) = \rho_\uparrow(k) - \rho_\downarrow(k)$. The (cross) charge-spin correlations, measured by $S_{nm}(k)$, need not be considered since they exactly vanish in the paramagnetic fluid.

The building up of a quasi-crystalline order with increasing the coupling is clearly seen in our DMC results shown in Fig. 2 for $b = a_B^*$. The static structure factor $S_{nn}(k)$, while very close to the Hartree-Fock prediction at $r_s = 1$, with increasing $r_s$ develops a pronounced peak at $4k_F$, which in fact may be shown to be divergent with the number of particles $N$, for large couplings, (see below). A pronounced peak at $4k_F$ corresponds in real space to slowly decaying oscillations, with period equal to the average interparticle distance $2r_sa_B^*$, thus suggesting quasi-crystalline order. In the same figure we also give the predictions of approximate theories such as STLS or its dynamical version [24] (DSTLS). The STLS only gives the lowering of $S_{nn}(k)$ at small and intermediate values of $k$, for increasing $r_s$, but fails completely in yielding a peak. On the contrary, the DSTLS prediction develops a peak, with increasing the coupling, though its position is off by about 20%; the height of the peak happens to almost coincide with that of the DMC result at $N=22$. Similar DSTLS results were recently obtained for a slightly different model of wire [25]. We should mention that at the time of writing we were not able to obtain a solution to DSTLS for $r_s > 6$.

Recently, Schulz analyzed the properties of a yet different wire with long range interactions also behaving as $e^2/\epsilon|x|$ at large $x$, resorting to a linearized dispersion of the kinetic energy and employing the bosonization technique [23], which gives exact results for a a Luttinger liquid [8]. He found persistent tails in the pair correlations, both for the number and magnetization variables, implying a divergent peak in the number structure factor $S_{nn}(k)$ at $4k_F$, and a pronounced but finite peak in the magnetization structure factor $S_{mm}(k)$ at $2k_F$. In his prediction, however, real-space tails contain undetermined interaction-dependent prefactors.

As we found that at $N = 22$ our DMC and variational Monte Carlo (VMC) results for the structure compare fairly well with each other [19, 24], we have employed VMC to study the $N$ dependence of the peaks of the structure factors, which we shown in Fig. 3. In passing, we mention that our VMC results for the paramagnetic fluid almost coincide with those obtained from a harmonic treatment of
a finite linear chain. It is evident that, at variance with the results for the Luttinger liquid, we have indication of peaks diverging with $N$ only at large values of the coupling, but for both $S_{nn}(k)$ and $S_{mm}(k)$. In addition $S_{mm}(2k_F)$ appears to grow faster with $N$ than $S_{nn}(4k_F)$, again in contradiction with the results of Ref. [23]. Possible explanation of these differences might be traced to either the undetermined interaction dependent prefactors mentioned above or to the fact that in the present study the full dispersion of the kinetic energy was retained.

4. CONCLUSIONS AND ACKNOWLEDGEMENTS

We have presented accurate results for one-dimensional electron gases adapted to describe quantum wires of different width, focusing on the energy and the pair correlations. Our results for the energy, which are exact, do no involve surprises: they satisfy the Lieb-Mattis theorem, in contrast to approximate treatments[16, 26], and rule out the occurrence of a Bloch instability. Thus, the origin of the anomalous plateau observed in the conductance of GaAs quantum wires, in the limit of single channel occupancy[10], should be sought elsewhere.

Our results for the pair correlations, on the other hand, are intriguing. They are not exact. Yet they should be rather accurate and is natural to make comparison with the predictions for the Luttinger liquid studied by Schulz[23], which has a slightly different interparticle interaction but with same long range tail. However, as we have observed above, it does not appear possible to reconcile in a simple manner the predictions of the present investigation with those of Ref. [23]. One possibility could be that the unknown interaction-dependent constants entering the tails of the pair correlations of the Luttinger liquid could in fact have a singular dependence on the coupling. At this time, we can only say that this issue deserves further investigations, both with bosonization techniques, to fully determine the coupling dependence of the tails in the pair correlations, and with numerical simulations, to estimate structure factors in an exact fashion. To this end one might resort to the recently proposed reptation Monte Carlo[27], which provides a simple direct way to evaluate ground state averages of local operators exactly.

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