Spin and charge Tomonaga-Luttinger parameters in quantum wires

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Abstract. – Low-energy properties of the homogeneous electron gas in one dimension are completely described by the group velocities of its charge (plasmon) and spin collective excitations. Because of the long range of the electron-electron interaction, the plasmon velocity is dominated by an electrostatic contribution and can be estimated accurately. We report on Quantum Monte Carlo simulations which demonstrate that the spin velocity is substantially decreased by interactions in semiconductor quantum wire realizations of the one-dimensional electron liquid.

The homogeneous electron liquid (HEL), historically important [1] as a simple model of a metal, continues to be of interest both in three dimensions (3D) [2] and in systems of reduced dimensionality. The quantum ground state of this model system is determined by a competition between kinetic and interaction energies, and depends only on r_s, the radius in atomic units of a sphere containing one electron. When the density is high ($r_s \lesssim 1$), the ground-state energy and, more interestingly, the parameters which characterize the system's low-energy excitations, can be evaluated using semi-analytic perturbative techniques [3]. At lower densities (larger r_s), correlations are strong and numerical Quantum Monte Carlo (QMC) calculations are required [4].

Unlike their higher-dimensional counterparts, 1D interacting fermion systems are not Fermi liquids; instead they exhibit the low-energy phenomenology common to many 1D fermion systems, often referred to as Tomonaga-Luttinger (TL) liquids [5,6]. Any TL liquid is completely specified by four parameters: the charge and spin collective excitation velocities v_ρ and v_σ, and the correlation exponents K_ρ and K_σ. In the absence of interactions v_ρ and v_σ reduce to the Fermi velocity, v_F, and the correlation exponents are equal to 1. Many quantities of immediate physical relevance can be expressed in terms of the TL parameters [6].

Symmetry and other considerations can reduce the number of independent TL parameters. The Galilean invariance of continuum models simplifies the charge sector, since the product [7] $v_\rho K_\rho = v_\mathrm{F}$ is not altered by interactions. Spin-rotational invariance simplifies the spin-sector since it requires $K_\sigma = 1$ [6]. The low-energy physics of the HEL is thus specified by v_ρ and v_σ.

In this letter we use QMC simulations to estimate, for the first time, v_ρ and v_σ [8] for a model which includes realistic long-range interactions [9]. The values we find for v_ρ in typical experimental circumstances are consistent with the large enhancements predicted perturbatively. Confirming this relation is important for a microscopic understanding of the exponents deduced from power laws in the transport properties at finite voltages or temperatures [10]. In the spin sector most works leave v_σ unspecified, or assume that v_σ would not deviate much from v_F. Taking the model originally proposed by Luttinger [11] with left- and right-going particles treated as distinguishable, the spin velocity indeed stays unrenormalized, $v_\sigma = v_\mathrm{F}$ [12]. Reliable knowledge of v_σ is vital to understand the operation of devices where spin instead of charge is transported [13], such as the "spin transistor" [14]. We find that v_σ is not described well by perturbative estimates, and, contrary to common wisdom, is strongly reduced by interactions.

The 1D HEL [15, 16] is realized in semiconductor systems with carriers electrostatically or chemically confined along a line, and with densities sufficiently low to quantize transverse motion, *i.e.* to realize the single-channel limit of a quantum wire. In 1D, the singularity of the $1/r$ repulsive interaction between electrons is cut off at short distances by the transverse width d of the lowest subband wave function. Usually the interaction is also cut off at large distances R due to screening by mobile external electrons in gates which help to define the electron channel. We use the form

$$V(|x|) = e^2 \left(\frac{1}{\sqrt{x^2 + d^2}} - \frac{1}{\sqrt{x^2 + d^2 + 4R^2}} \right) \tag{1}$$

for the electron-electron interaction as suggested by a static image charge model of remote screening by 3D metals. We consider a system to be a 1D HEL provided that $R \gg r_\mathrm{s} a_\mathrm{B}$, where a_B is the host semiconductor Bohr radius. In 1D r_s is related to the density by $n = 1/(2 r_\mathrm{s} a_\mathrm{B})$, and has to exceed a minimum value $r_\mathrm{s}^\mathrm{min}$ to suppress higher subband occupations. For a parabolic transverse confining potential $r_\mathrm{s}^\mathrm{min} = (\pi/4\sqrt{2})(d/a_\mathrm{B}) \sim 0.55(d/a_\mathrm{B})$. Values of d/a_B and R/a_B for a particular sample can be estimated from measured subband energy separations and the sample layout, respectively. For the numerical calculations described below, we use $d = 0.5 a_\mathrm{B}$ and $R = 7.07 a_\mathrm{B}$. This value of d is probably somewhat smaller than that which can be achieved at present in samples where interactions dominate disorder, while the value of R is somewhat smaller than a typical one, since we want to study the crossover to short-range interaction physics which occurs when r_s exceeds R/a_B.

For the QMC simulations a lattice representation

$$H = -\frac{\hbar^2}{m^* L^2} \frac{M^2}{2} \left[\sum_{\sigma \langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{h.c.}) - 2N \right] + \sum_i V_{ii}\, n_{i\uparrow} n_{i\downarrow} + \sum_{i<j} V_{ij}\, n_i n_j \tag{2}$$

is particularly convenient for the use of a standard "world-line" QMC algorithm [17]. The number of lattice points used in our simulations ranged from $M = 32$ to $M = 64$ on a chain of length L (with periodic boundary conditions), while 960 time slices divided the Trotter axis. The inverse temperature, β, was set to a high value, $\beta = 96 m^* L^2/M^2$, to ensure that the ground-state properties were sampled. The continuum limit and the quadratic single-particle spectrum are recovered at particle numbers $N \ll M$. In eq. (2) $V_{ij} = V(L|i-j|/M)$.

To verify our procedures for extracting the TL parameters from the QMC data, we first examined the case of the Hubbard model where v_σ and v_ρ are known exactly [9] from the Bethe ansatz solution [18]. The Hubbard limit is readily obtained from (2) by setting $V_{ij} = 0$ for $i \neq j$, and identifying the prefactor of the first term with the hopping t and V_{ii} with the on-site Hubbard repulsion U. The velocities v_σ and v_ρ may be obtained most directly from the QMC data by calculating the dispersion relations for spin and charge excitations. A method proposed by Yamamoto [19] was found to give high-quality results which could be further checked against alternative numerical analytic continuation methods such as the Maximum Entropy [20] or SVD [21] methods. The Luttinger liquid relations themselves can also be used to derive v_σ and v_ρ from the thermodynamic quantities, the compressibility and the uniform susceptibility [6], which can be evaluated to a high degree of accuracy by QMC. Both approaches gave high-quality estimates for v_ρ. The results for v_σ were, however, considerably noisier, and at large values of U neither method was able to reliably resolve very small spin velocities. As the results derived from the susceptibility agreed significantly better with the exact v_σ [22], we used this method to obtain the results presented below, and used the dispersion relation methods as additional checks.

Figure 1 shows the ground-state energy density E_0 of (2) *vs.* $k_\mathrm{F}d = \pi(d/a_\mathrm{B})/4r_\mathrm{s}$ in units of $\varepsilon_0(k_\mathrm{F}) = E_0 m^*/k_\mathrm{F}^3$ (k_F is the Fermi momentum). Without interactions $\varepsilon_0(k_\mathrm{F}) = 1/3\pi \sim 0.106$. The results are based on 4000 samples, drawn from $\sim 10^5$ configurations. To rule out ergodic "sticking", we compared different starting configurations, and found that in all cases the energies converged to the same values within statistical errors. A careful finite-size scaling analysis for E_0, based on the conformal symmetry result [23] $E_0(L) = E_0(L = \infty) - c/L^2$, fitted the simulation data extremely well.

Since a full finite-size analysis for every value of $k_\mathrm{F}d$ would be too time consuming, we chose instead to estimate the corrections by interpolating linearly between the finite-size corrections obtained at $k_\mathrm{F}d = 0.079$ ($r_\mathrm{s} = 4.97$) and $k_\mathrm{F}d = 0.5$ ($r_\mathrm{s} = 0.78$). Additional finite-size analyses at $k_\mathrm{F}d = 0.132$ and $k_\mathrm{F}d = 0.314$ confirmed the accuracy of this interpolation.

In fig. 1 the first-order perturbation (Hartree-Fock) theory result $\varepsilon_0^{\mathrm{pert}} = \frac{1}{3\pi} + \frac{2}{\pi^2 v_\mathrm{F}}\hat{V}(0) - \frac{1}{2\pi^2 v_\mathrm{F} k_\mathrm{F}^2}\int_0^{2k_\mathrm{F}} \mathrm{d}k\ (2k_\mathrm{F} - k)\hat{V}(k)$ is also shown, which establishes an upper bound to the ground-state energy due to its variational nature. Here $\hat{V}(k)$ is the Fourier transform of the interaction (1).

We further include in fig. 1 the harmonic lattice approximation to the energy of an electron crystal state:

$$E_0^{\mathrm{wc}} = E_0^{\mathrm{cl}} + \frac{1}{2}\int_{-k_\mathrm{F}}^{k_\mathrm{F}} \frac{\mathrm{d}k}{2\pi}\ \omega(k)\,, \tag{3}$$

where $E_0^{\mathrm{cl}} = \frac{1}{2L}\sum_{i\neq j} V(|i-j|/n)$ is the classical energy and $\omega^2(k) = \frac{1}{m^*}\sum_{j=1}^{\infty} V''(j/n)(1 - \cos jk/n)$ is the dispersion of harmonic fluctuations. Primes denote derivatives with respect to the arguments. E_0^{wc} sets a lower bound to the true ground-state energy since the quartic term of the Coulomb interaction is positive when expanded as a power series, and since spin is ignored in (3). We see in fig. 1 that in the high-density regime, where the electrostatic term $\hat{V}(k = 0)$ dominates the energy, the ground-state energy is bounded within a narrow interval. At smaller densities, when $r_\mathrm{s}a_\mathrm{B} \gtrsim R$, we cross over to the short-range interaction regime where the Hartree-Fock (HF) estimate fails especially badly.

The most striking result of this work, the spin-velocity TL parameter, is presented in fig. 2. As mentioned, this quantity was calculated using the TL theory expression [6] $\chi(q \to 0, \omega = 0) = (2/\pi)K_\sigma/v_\sigma$, with $K_\sigma = 1$. The susceptibility χ can be extracted from the simulations by

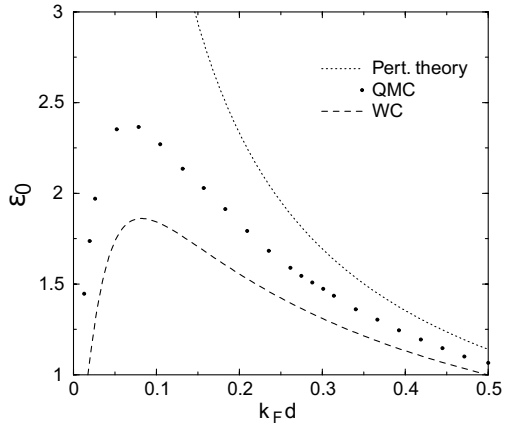

Fig. 1

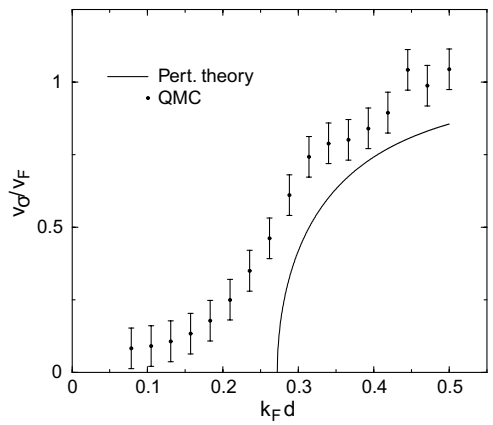

Fig. 2

Fig. 1 – QMC dimensionless ground-state energy density ($\varepsilon_0 = E_0/v_\mathrm{F}k_\mathrm{F}^2$) of quantum wires *vs.* $k_\mathrm{F}d$ for $R/d = 14.14$ and $d/a_\mathrm{B} = 0.5$. Also included are the Hartree-Fock (dotted line) and harmonic (dashed line, cf. eq. (3)) approximations to the energy.

Fig. 2 – Spin velocity, normalized to the Fermi velocity. The perturbative result is given by the solid line.

integrating the QMC Matsubara spin-density–spin-density correlation function over imaginary time. In the same way, the compressibility $\kappa = (2/\pi)(K_\rho^2/v_\mathrm{F})$ can be derived from the density-density correlation function, and the values for κ calculated in this manner agree with those obtained from the ground-state energies (see below), and also with those obtained from charge dispersion relations, confirming again the reliability of extracting TL parameters from susceptibilities. Similarly to the case of the Hubbard model, the spin correlation function was found to be considerably noisier than its density counterpart, particularly at lower particle densities where correlations are stronger. As a result, the spin data are subject to larger statistical errors. The QMC estimate can be compared with the perturbative generalized-random-phase approximation [24], $v_\sigma^\mathrm{GRPA}/v_\mathrm{F} = (1 - \hat{V}(2k_\mathrm{F})/\pi v_\mathrm{F})^{1/2}$, also shown in fig. 2. The GRPA spin-velocity goes to zero as the ferromagnetic instability predicted by the HF energy approximation is approached. (This occurs at $r_\mathrm{s} \sim 1.44$ for $d = 0.5a_\mathrm{B}$.) In 2D [25] the instability occurs at $r_\mathrm{s} = \pi/\sqrt{2} \sim 2.22$, and in 3D [1] at $r_\mathrm{s} = (9\pi^4/4)^{1/3} \sim 6.03$.

Ferromagnetic instabilities predicted by the HF approximation have provided an important motivation for the Monte Carlo calculations in higher dimensions, where it has been established [2, 4] that the transition does not occur until substantially larger r_s values are reached, if at all. In 1D the Lieb-Mattis theorem [26] guarantees that the ferromagnetic transition does not occur at any r_s, in disagreement with conclusions based on recent density-functional calculations [27], which give results similar to the HF approximation results quoted here. Nevertheless, this instability may be taken as a marker for the crossover from weak to strong correlations which, we note, occurs at substantially smaller values of r_s in reduced dimension systems.

For the quantum wire system [15] of Yacoby *et al.*, we estimate $d/a_\mathrm{B} \sim 0.7$ and take the "typical" density to be one fifth of that at which the second subband is occupied. This corresponds to $r_\mathrm{s} \sim 1.93$ and $k_\mathrm{F}d \sim 0.28$, close to the value at which ferromagnetism is predicted in the HF approximation. Near this density, our QMC calculations show a paramagnetic state,

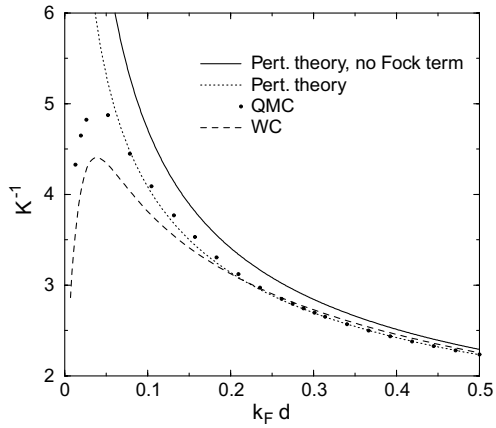

Fig. 3 – K_ρ^{-1} *vs.* $k_{\rm F}d$. The same approximations are included as in fig. 1 and in addition the result without the negative exchange term in (4).

albeit one with v_σ reduced by a factor of more than two compared to $v_{\rm F}$. At this density, the fractional spin-polarization $\xi = (S(\xi)r_{\rm s}^2/2)(g\mu_{\rm B}B)/(\hbar^2/2m^*a_{\rm B}^2)$ produced by laboratory fields ($\xi \sim 0.2$ at $B = 20$ tesla in GaAs) is considerably increased by the spin enhancement factor $S(\xi)$ due to interactions (for $\xi \to 0, \quad S(\xi) = v_{\rm F}/v_\sigma$). Such reduced magnetic stiffness, due to correlations which keep electrons apart, will lead to substantial spin-polarization in quantum wires at routinely available magnetic fields. This may play a role in quantum transport experiments, like those of Thomas *et al.* [28].

Spin velocities can be measured using inelastic light scattering in depolarized configuration [29] or, in principle, with ferromagnetic contacts attached [13], using time-resolved techniques [30]. Indeed, the Raman data obtained by Goñi *et al.* [31] indicate clearly smaller values for v_σ compared to $v_{\rm F}$.

In closing we discuss the charge physics of semiconductor quantum wires. The TL relation $K_\rho^{-2} = \frac{\pi}{2}[k_{\rm F}^2\varepsilon_0''(k_{\rm F}) + 6(k_{\rm F}\varepsilon_0'(k_{\rm F}) + \varepsilon_0(k_{\rm F}))]$ enables very accurate estimates to be made for $v_\rho = v_{\rm F}/K_\rho$, since thermodynamic quantities converge more rapidly than dynamical ones during the QMC simulations, and can also be corrected for finite-size effects more easily. The QMC energies were smoothed by a cubic spline fit to avoid amplifying any small irregularities in the stochastic data in performing the numerical differentiation.

In fig. 3 the thus obtained values for K_ρ (describing correlation functions up to logarithmic prefactors [32]) are compared with GRPA and harmonic lattice values. The GRPA compressibility is obtained from the corresponding HF energy expression which leads to

$$K_\rho^{\rm GRPA} = [1 + (2\hat{V}(k=0) - \hat{V}(k=2k_{\rm F}))/\pi v_{\rm F}]^{-\frac{1}{2}}. \tag{4}$$

We see that eq. (4) fits the QMC values well, down to quite small particle densities, which is unexpected in view of the possible renormalization of K_ρ at small energies. Only at $r_{\rm s} \gtrsim R/d$, where $1/K_\rho^{\rm GRPA} \propto v_{\rm F}^{-1/2} \propto \sqrt{r_{\rm s}}$, does GRPA fail to reproduce the maximum seen in the QMC data and in $1/K_\rho^{\rm wc}$. Finally, at very small densities, $k_{\rm F} < d/R^2$, the harmonic approximation $K_\rho^{\rm wc} \sim k_{\rm F}^{-1/4}$ also fails, underestimating the residual kinetic energy and violating the condition that $K_\rho < 1$ for repulsive interactions. It has been conjectured that $K_\rho \to 1/2$ as $k_{\rm F} \to 0$ for any finite-range interaction [33], which is consistent with the value obtained by extrapolating the QMC data to $k_{\rm F} \to 0$.

Close inspection of the QMC data in fig. 3 reveals that $1/K_\rho$ actually *exceeds* the perturbative estimate before it levels off towards the maximum at decreasing $k_{\rm F}$. In this regime the system is clearly stiffer than perturbation theory suggests. Such behavior is also known from higher dimensions, where the inverse compressibility is underestimated by the GRPA. A larger value of R would enlarge this regime of densities, and make this enhancement even more pronounced.

In conclusion, by means of QMC we have found that spin velocities in typical experimental realizations are significantly reduced by interactions, enhancing the instability with respect to ferromagnetism. This finding is of direct relevance to "spintronic" devices using the HEL. Furthermore, we have established the regime of validity of the widely used perturbative expression for the charge correlation exponent K_ρ, and found a clear non-monotonic dependence on carrier density.

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