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Tunneling exponents in realistic quantum wires using the mean field approximation

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Interacting carriers in one dimension (1D) are non-Fermi liquids with power laws for many correlations functions such as the tunneling density of states. Evidence for this behavior has been found in carbon nanotubes[1)] and, somewhat less convincingly, in semiconducting quantum wires[2)] in the form of non-trivial temperature and transport voltage dependences. Non-universal exponents are expressed through one parameter K_ρ within the Tomonaga-Luttinger (TL) liquid theory.

In Fermi-liquids K_ρ equals unity. This quantity is commonly expected to decrease with increasing repulsion V_0 between the carriers, according to

$$K_\rho = [1 + 2V_0/\pi v_{\rm F}]^{-1/2} \, . \tag{1}$$

Eq. (1) results also from the RPA-approximation for the 1D-plasmon velocity[3)] which has shown to be exact for spinless carriers and for strictly linear kinetic energy dispersion.[4)] Eq. (1) implies that $K_\rho \to 0$ with decreasing carrier density $n = 2k_{\rm F}/\pi = 2mv_{\rm F}/\pi$ for quadratic kinetic energy dispersion $\sim k^2/2m$ when $v_{\rm F} = k_{\rm F}/m$.[5)]

For given microscopic interaction potential $V(x)$, where the Coulomb form in any realistic sample layout will be screened by the nearest metals at a distance R, does K_ρ depend on the carrier density in a non-monotonous fashion, passing through a minimum before reaching the asymptotic value which was conjectured to be $K_\rho(n \to 0) \to 1/2$.[6)] Observing this minimum could give direct experimental access to the range of the microscopic interaction. We shall argue that the value of K_ρ can be obtained quite accurately by the Hartree-Fock approximation when augmenting selfconsistency (SCHF).

As a realistic form modeling the microscopic interaction in a quantum wire of width d at particle separation $|x - x'|$ we use

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

with $V(|x-x'| \gg R) \sim |x-x'|^{-3}$, describing dipolar screening. We have solved the Hartree-Fock equations for a system of length L, accounting for the quadratic kinetic energy dispersion and for spin $s = \pm$

$$0 = \left[\frac{1}{2}(2j - \frac{k}{k_{\rm F}})^2 - \frac{\varepsilon_{ks}}{k_{\rm F} v_{\rm F}}\right] u_{j,k,s} \tag{3}$$

$$+ \frac{L}{2k_{\rm F}\pi} \sum_{j'j''} u_{j'',k,s} \int_{-k_{\rm F}}^{k_{\rm F}} {\rm d}k' \left\{ \hat{V}\Big(2(j-j'')\Big) \times \sum_{s'} u^*_{-j+j'+j'',k',s'} \, u_{j',k',s'} - \hat{V}\Big(2(j-j') - \frac{k}{k_{\rm F}} + \frac{k'}{k_{\rm F}}\Big) \, u^*_{-j+j'+j'',k',s} \, u_{j',k',s} \right\}$$

selfconsistently in k-space for the coefficients $u_{j,k,s}$ $(-k_{\rm F} \le k \le k_{\rm F})$ that expand the HF-orbitals (index j) as Bloch waves

$$\psi_{ks}(x) = {\rm e}^{{\rm i}kx} \sum_j u_{j,k,s} \, {\rm e}^{{\rm i}j2k_{\rm F}x} \, . \tag{4}$$

Resulting total ground state energy densities $E_0^{\rm HF}/L$ are differentiated twice w.r.t. n to obtain the HF-estimate to the compressibility $\kappa = [\partial^2(E_0/L)/\partial n^2]^{-1}$. Using the exact thermodynamic relationship

$$K_\rho = \sqrt{\pi v_{\rm F} \kappa / 2} \tag{5}$$

from TL-theory[7)] yields $1/K_\rho^{\rm HF}$, shown in Fig. 1. Also included in Fig. 1 are quantum Monte Carlo data taken from Ref.[8)] that, within symbol size, can be regarded as exact. It is seen that $K_\rho^{\rm HF}$ does reproduce all of the available QMC-data points amazingly well. In view of the pronounced correlations of interacting one-dimensional Fermions, which prohibit for example to express the ground state wave function analytically, such a quite satisfying mean-field approach might seem unexpected.

The following general trends are seen in Fig. 1:
(*i*) The high density region $k_{\rm F}d \gtrsim 0.25$, corresponding to $r_{\rm s} \lesssim 1.6$, may be regarded as the perturbational or RPA regime. Here Eq. (1) may be improved slightly by accounting for the exchange contribution $\sim -\hat{V}(2k_{\rm F})$. Despite of the quite small values of K_ρ estimated[9)] and observed[1)] in carbon they nanotubes belong typically to this regime, since mean carrier separations exceed by far the interaction range (which can reach the order of the tube length).
(*ii*) Between $0.1 \lesssim k_{\rm F}d \lesssim 0.25$ the perturbational expression still allows to guess K_ρ. Here, particularly the SCHF but also the QMC-data indicate slightly enhanced K_ρ^{-1}-values, relative to Eq. (1). By virtue of (5) this suggests a *reduced* compressibility which can be interpreted as precursor to a Wigner crystal phase transition (that cannot be completed in 1D). There, K_ρ has been esti-

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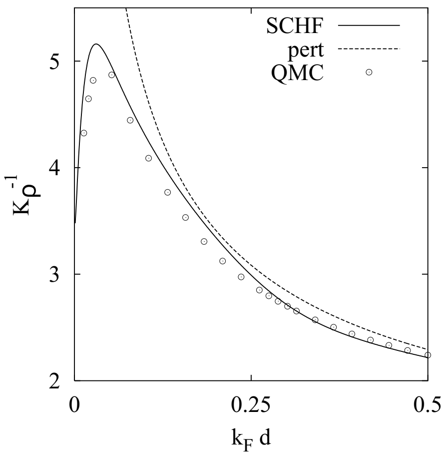

Fig. 1. K_ρ^{-1} versus carrier density. The units can be translated into the r_s-Fermi liquid parameter using $r_s = \pi/8k_F d$. The range of the microscopic interaction (2) is $R/d = 14.1$. Solid: self consistent HF approximation, dashed: Eq. (1). QMC-data are taken from Ref.[8)]

mated first in.[10)]
(*iii*) Finally, for the interaction range $R/d = 14.1$ shown in Fig. 1, a maximum is seen below $k_F d \lesssim 0.1$ ($r_s \gtrsim 4$) in both, the SCHF and the QMC results, in qualitative difference to the monotonous increase of the perturbative expression (1). This maximum occurs roughly when $k_F R \approx \pi/8$ (R has to be significantly smaller than the mean carrier spacing due to quantum fluctuations). In semiconducting quantum wires this regime (*iii*) should be feasible.

It has been conjectured that $1/K_\rho$ would approach 2 when $k_F \to 0$.[6)] This limit is not confirmed by the SCHF which, when carried out carefully to account for the pronounced $4k_F$-periodic oscillations of the SCHF-density (resembling a Wigner crystal), yields $1/K_\rho^{\rm HF} \to 3.3$ with a weak dependence on R/d, ranging from $1/K_\rho^{\rm HF} \to 3.0$ at $R/d = 5.7$ to $1/K_\rho^{\rm HF} \to 3.5$ at $R/d = 35$. Unfortunately, the QMC-data cannot discriminate between $1/K_\rho \to 2$ and $1/K_\rho \to 3.5$. This discrepancy might indicate the failure of the mean field approximation to estimate K_ρ in the strongly correlated regime of very small carrier densities.

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