Ladder approximation to spin velocities in quantum wires

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The spin sector of charge-spin separated single mode quantum wires is studied, accounting for realistic microscopic electron-electron interactions. We utilize the ladder approximation (LA) to the interaction vertex and exploit thermodynamic relations to obtain spin velocities. Down to not too small carrier densities our results compare well with existing quantum Monte-Carlo (QMC) data. Analyzing second order diagrams we identify logarithmically divergent contributions as crucial which the LA includes but which are missed, for example, by the self-consistent Hartree-Fock approximation. Contrary to other approximations the LA yields a non-trivial spin conductance. Its considerably smaller computational effort compared to numerically exact methods, such as the QMC method, enables us to study overall dependences on interaction parameters. We identify the short distance part of the interaction to govern spin sector properties.

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At low energies the one-dimensional (1D) electron liquid exhibits charge-spin separation\(^{12}\), in contrast to the Fermi liquids of higher dimensionality\(^{3}\). Theoretical considerations based on the Tomonaga-Luttinger liquid (TLL)\(^{4}\) have predicted this behavior\(^{5}\) and recent experiments\(^{6,7}\) has provided strong evidence supporting different velocities \(v_\sigma\) and \(v_F\). Both velocities differ from the Fermi velocity \(v_F\) in the Hubbard model, for example, charge density waves (plasmons) propagate faster, \(v_\rho > v_F\), while spin density waves propagate slower, \(v_\sigma < v_F\), than the Fermi velocity for repulsive on-site interaction\(^7\).

Quantitative knowledge of \(v_\sigma\) is decisive to predict spin transport\(^8\) and magnetic properties\(^9\). Within the random phase approximation (RPA), or when treating left and right going particles as distinguishable\(^{10,11}\) as originally done by Luttinger\(^{12}\), \(v_\sigma = v_F\) stays unrenormalized with interactions\(^{13}\). On the other hand, even in first order perturbation theory the exchange or Fock term, proportional to the \(2k_F\)-Fourier component of the electron-electron interaction \(V(q)\), influences the spin velocity. (In contemporary quantum wires the range of the interaction usually exceeds the Fermi wavelength, so \(V(q=0) \neq V(q=2k_F)\)). Quantitatively, however, this latter approach is limited to \(V(2k_F) \ll v_F\) (corresponding to electron gas parameters \(r_s \ll 1\)). Furthermore, it spoils SU(2) spin rotation invariance of the microscopic electron model, see below. Quantum Monte Carlo (QMC) has demonstrated that \(v_\sigma/v_F\) decreases with increasing inter-particle repulsion in quantum wires\(^{14}\), in qualitative resemblance to the Hubbard model\(^{15}\). Values of \(v_\sigma/v_F \approx 0.5\) have been estimated\(^{13}\) for present day single channel quantum wires\(^{14,15,16}\).

Numerically exact techniques, however, are computationally extremely demanding, especially in spin sector. This yet has prohibited scans through larger parts of the parameter space that characterizes the microscopic interaction; in Ref.\(^{13}\) only one interaction range and one channel width has been investigated. A future study of multi-channel quantum wires would require using considerably bigger systems. Here, a sufficiently accurate and tractable approximative scheme would be helpful. Among the techniques established for Fermi liquids the Hartree-Fock approximation (HF) has proven as useful to estimate boundary exponents\(^{17}\) and, when carried out self-consistently, to yield amazingly quantitative results in charge sector\(^{18}\). It captures for example very well the non-monotonous dependence of \(K_\rho\) on the electron density\(^{19}\), beyond the RPA. On the other hand, the mean field approximation has turned out to fail badly in spin sector\(^{20}\). Below we show that in a perturbative language this failure can be traced back to the wrong class of diagrams summed by the self consistent HF. In the present work we sum up ladder diagrams and demonstrate that they comprise a ‘complementary’ class of diagrams that account much better for spin properties.

The ladder approximation (LA) to the effective interaction vertex originally has been established to study strongly correlated fermion systems with short range interactions, such as nuclear matter\(^{21}\) but it performs remarkably well for the also strongly correlated charge sector of a 1DES\(^{22}\).

In comparison to other Fermi-liquid methods\(^{22}\), such as the Singwi, Tosi, Land, and Sölander (STLS) approximation scheme\(^{23,24,25}\), the LA is known to account well for short distance properties of the interaction when tested\(^{26}\) with exactly solvable models\(^{22}\). As we shall demonstrate, this short distance behavior is indeed most relevant to magnetic properties. In this paper we generalize the LA to allow for non-zero magnetizations and for spin currents to gain homogeneous and static spin susceptibilities. Summing ladder diagrams yields estimates to \(v_\sigma\) that compare well with existing QMC-data at not too low electron densities while the numerical effort stays com-
parable to self consistent HF calculations. This enables
us to scan different parameters of the microscopic inter-
action. Of prime interest, e.g. to carbon nanotubes are
the interaction range and the diameter of the quantum
wires.

I. MODEL

To model the microscopic interaction we use

\[ V(q) = \frac{2\nu_F}{k_F a_B} \left[ K_0(qd) - K_0(q\sqrt{d^2 + 4R^2}) \right] \] (1)

in momentum space, where \( K_0 \) denotes a modified Bessel
function and \( a_B \) is the Bohr radius. This form accounts
for the experimentally important parameters, the inter-
action range \( R \), given by the distance to the nearest metal
gate, and the diameter \( d \) of the wire, which determine
\( V(q) \) at small and at large \( q \), respectively. Details of the
wire’s cross section affect the interaction only at \( q > d^{-1} \),
i.e. at carrier densities where occupation of higher sub-
bands starts. We do not consider this case here.

In Fermion representation the quantum wire (length
\( L \), \( s = \pm 1 \) denotes spin) is described by

\[ H = \sum_{k,s} \epsilon(k) c_{k,s}^\dagger c_{k,s} + \]
\[ + \frac{1}{2L} \sum_{k,s,k',s',q} c_{k-q,s}^\dagger c_{k'+q,s'}^\dagger V(q)c_{k',s'} c_{k,s} \] (2)

\( c_{k,s} \) are Fermi operators in the wave number basis. For
non-linear single particle dispersion \( \epsilon(k) = k^2/2m \), as in
semiconducting quantum wires of effective carrier mass \( m \)
and in the presence of \( 2k_F \)-scattering between antiparallel
spins near opposite Fermi-points bosonization of model
introduces terms of higher than quadratic order in the
Bosonic density fluctuations. One could attempt, at
least in principle, to eliminate higher order terms by the
RG method in course of which they would renormalize all
pre-factors of the quadratic terms, \( \nu_F \), and interaction
are real as a consequence of the Lehmann representa-
tion of SU(2) invariance. The STLS only allows to calculate magnetic
susceptibilities in terms of the self-energy

\[ \Sigma_s(k,\omega) = G_s^0(k,\omega)^{-1} - G_s(k,\omega)^{-1} \] (6)

\( G_s(k,\omega) \) is the full electron propagator with respect to \( \nu_F \) and
\( G_s^0(k,\omega) = (\omega - k^2/2m + \text{sign}[(k - sI) - (k_F + sP)^2]i0)^{-1} \)
the free propagator. The ground state energy, required in
\( G_s \), can be expressed as

\[ E_0/L = \sum_s \frac{1}{4\pi^2} \int dk d\omega \left( \frac{k^2}{2m} + \omega \right) G_s(k,\omega) \] (7)

which reduces to

\[ E_0/L = \sum_s \frac{1}{2\pi} \int \frac{dk}{-k_F + s(I - P)} \left[ \frac{k^2}{2m} + \frac{1}{2} \Sigma_s(k) \right] \] (8)

for self energies not depending on frequency \( \omega \) (and there-
are real as a consequence of the Lehmann representa-
tion of \( G_s \)). This condition is fulfilled within the HF (cf.
Eq. 4 below) and within the LA. We are not aiming to
determine temporal or spatial correlation functions in the
Fermionic representation, but rely here on the exact solution \( \langle \Sigma \rangle \) of the Boson model.

It can serve as a test to the quality of any approxi-
mative scheme in spin sector whether or not it respects the
condition \( \nu_{N\sigma} = \nu_{J\sigma} \) dictated by SU(2) invariance.
The HF, for example, leaves \( \nu_{I\sigma} = \nu_F \) independent of in-
teractions since it ignores \( 2k_F \)-interactions between ele-
trons of opposite spins and thus violates spin rotation
symmetry. The STLS only allows to calculate magnetic
susceptibilities \( \nu_{N\sigma} \) in spin sector \( \langle \Sigma \rangle \), so it cannot be tested
in its behavior regarding the SU(2) symmetry. The LA finally does indeed renormalize $v_{J\sigma}$, though only by about half the amount it renormalizes the value for $v_{N\tau}$ compared to $v_p$. In so far we find that the LA does not fully obey the SU(2) symmetry but proves as superior to the other approximative schemes.

II. LADDER APPROXIMATION

To introduce the LA we follow the References 20 and 21 but generalize the calculations for finite magnetization $P$ and spin current $I$. The self-energy shift

$$\Sigma_s(k; P, I, k_p) = \frac{1}{2\pi} \sum_s \int \frac{dk'}{2\pi} \left[ g_{ss'}(k, k', 0) - \delta_{ss'} g_{ss'}(k, k', k - k') \right]$$

(9)

due to interactions with the sea of other electrons is expressed in terms of an effective (Brueckner) interaction matrix $g_{ss'}(k, k', q)$. Knowing $g_{ss'}(k, k', q)$ exactly would yield the exact ground state energy through 5 and, by virtue of 5, the exact values for the TLL-velocities. The Brueckner interaction matrix is closely related with the static structure factor which often is exploited to investigate how the short range part of the interaction affects short distance correlations of one-dimensional electron liquids 21,22.

For the ladder approximation a Bethe–Salpeter integral equation

$$g_{ss'}(k, k', q) = V(q) + \frac{1}{2\pi} \int_{-\infty}^{\infty} dp \ g_{ss'}(k, k', p) \times K_{ss'}(k, k', p) V(q - p)$$

(10)

has to be solved, describing multiple scattering between electrons that otherwise propagate freely outside the Fermi sphere according to

$$K_{ss'}(k, k', p) = \frac{2m}{\Theta(|k - sI| - p) - k_{F_{ss'}}} \Theta(|k' - s'I + p| - k_{F_{ss'}})$$

$$\Theta(1 + p^2 - k^2 - k'^2)$$

(11)

In 12 we have defined spin dependent Fermi-momenta $k_{F_{ss'}} \equiv k_{F} + sP$ at finite magnetizations. We solve equation (11) for each pair of momenta $(k, k')$ and spins $(s, s')$ the Householder method after mapping the infinite range to $[0, \pi]$ by $p = k_F \cot \phi$ and discretizing $\phi_i = \pi(i - 1)/(N - 1)$. A value of $N = 150$ turned out as an optimal compromise between CPU time (increasing with $N^3$) and accuracy (the error in $q \sim N^{-2}$ due to the cusps of $g(k, k', q)$ at $q = 2k_F$). Only at strong interactions, when spin velocities drop below half of the Fermi velocity, we used $N = 250$. Finally, ground state energies are integrated via 5 and 10 using the trapezoid rule on a grid of 129 points over the interval $[-2k_F; 2k_F]$ which sufficed to accurately resolve the effects of small magnetizations.

The solution $g_{ss'}(k, k', q)$ exhibits pronounced dependence on $k$ and $k'$, cf. Figure 1 arising primarily from the short distance correlations at $k = -k'$. Ignoring this dependence, as it is commonly done in 3D (cf. Ref. 20 and references therein), would clearly not be justified. This correlation has similarities to the striking anti-ferromagnetic $2k_F$ modulations found in the self-consistent HF–density in 1D 13 which also cannot be ignored for reliable results in the charge sector.

III. RESULTS

Figure 2 shows ground state energies (in units of the respective kinetic energies) versus carrier density using different approximations. QMC data 13 can be regarded as exact within symbol size. Remarkably, at densities $k_Fd \gtrsim 0.2$, where self-consistency is seen in Figure 2 to still improve the HF–estimate to $E_0$ compared to ‘pert’
(and then provides the optimum Fermi–liquid wave function), the LA yields slightly lower ground state energies. As seen in Figure 3, the LA also yields better values of $K_\rho$ in this regime. Only at smaller electron densities HF-theory engenders lower ground state energies and a better estimate to the $K_{\rho'}$-parameter ($k_Fd < 0.1$). This energy gain is accompanied by spontaneous symmetry breaking and pronounced (though unreal) static $4k_F$–periodic Wigner crystal-like modulations\(^{19}\) of the charge density in the HF ground state. However, this success of the HF in charge sector does clearly not carry over to the spin sector\(^{18}\) as seen in Figure 4.

Remarkably, in the LA the spin velocity follows the QMC-data down to rather low electron densities, superior to other electron gas theory approaches. Only at small densities $v_{sL}^{LA}$ vanishes, pretending the transition into a ferromagnetic ground state which is not expected to occur in 1D for finite range interactions. The LA does not reproduce the behavior $v_\sigma \propto K_F^2$ derived from the Hubbard model at small fillings\(^{30}\) to which quantum wires should cross over\(^{19}\) when the inter-particle spacing exceeds the interaction range, $k_F R \ll \pi/2$.

Figure 5 demonstrates that at interaction ranges $k_F R \gg \pi/2$ the value of $R$ does not affect the spin velocity, unlike the ground state energy or the charge sector exponent which both depend logarithmically on $R/d$. This is consistent with the perturbative result according to which $V(k = 2k_F)$ but not $V(k = 0)$ governs the magnetic susceptibility where the former $V(2k_F) \sim 2V_F K_0(2k_F d)/k_F a_B$ becomes independent of $k_F R \gg 1$. This is of particular relevance to carbon nanotubes\(^{25}\) where $k_F R$ can be of the order of $10^3$. The inset of Figure 5 complements Figure 4, showing how the spin velocity varies with wire width $d$ at fixed $k_F d = 0.3$.

**IV. DISCUSSION**

To analyze further why the LA captures magnetic properties so well we compare it diagrammatically with the self-consistent HF. For this purpose we use the self-energy\(^{13}\) were HF and LA can be compared directly. We expand the self-energy\(^{14}\) to second order in the interaction. The first order contribution, obtained by putting $g(k, k', q) = V(q)$ in \(^{11}\), yields

$$\Sigma_{s,\text{pert}}(k + sI) = \frac{4k_F}{2\pi} V(0) - \frac{k_F + sP}{k_F - sP} \int \frac{dk'}{2\pi} \frac{V(k' - k')}{2\pi} .$$

(12)

The exchange term on the right hand side of (12) is effective only for parallel spins and therefore independent of the spin current $I$ so that $v_{s,\sigma}$ remains un-renormalized to this order.

Self-consistent HF is described by

$$\Sigma_{s,\text{HF}}(k) = -i \left( \frac{4\pi^2}{4\pi^2} \sum s' \left( V(0) - \delta_{ss'} V(k - k') \right) G_{s'}(k', \omega) \right) G_{s}(k, \omega)$$

(13)

$$G_s(k, \omega) = G_0^s(k, \omega) + G_0^s(k, \omega) \Sigma_{s,\text{HF}}(k) G_s(k, \omega)$$

(14)

To first order, $\Sigma_{s,\text{HF}}(k)$ agrees with (12). We see that \(^{13}\) will not depend on $I$, even when self-consistence $G^0 \rightarrow G$ is reached.
and the spin conductance 

\[ v \] magnetic susceptibility, 

\[ \partial \] at opposite Fermi points which affects 

\[ \text{scattering between antiparallel} \]

\[ \text{to} \]

(9) and (10) for the LA or (13) and (14) for the HF, 

\[ \text{describes scattering between antiparallel} \]

\[ b \]

(both of the approximations, insofar the LA and the HF 

These are all irreducible second order contributions.

Furthermore, only term (a) breaks Galilei invariance in spin sector as required to satisfy the SU(2) symmetry condition according to which the spin conductance should be equally renormalized by interactions as the magnetic susceptibility, 

\[ v_{\text{LA}} = v_{\text{HF}}. \]

Term (a) in (15) describes scattering between antiparallel \( s = -s' \) spins at opposite Fermi points which affects \( \partial_I \Sigma^{(2)}_s(k; P, I, k_F) \) and the spin conductance \( v_{J,s} \).

In order to compare the importance of the different terms (a) to (f) regarding \( \partial_P \Sigma^{(2)}_s(k; P, I, k_F) \) and thus the magnetic susceptibility \( v_{N,s} \) we consider for the moment a contact interaction, \( V(q) = V \). Then all second order contributions can be calculated analytically. The sum of all spin parallel parts \( s = s' \) cancel (spin parallel Fermions do not interact at contact) and only the \( s = -s' \) part of (a) and the term (c) (with \( s' = s \) or \( s' = s'' \)) remain non-vanishing. The latter is not divergent while term (a) can be expressed by sums of dilogarithms\(^{12}\) which can further be analyzed for \( I, P \ll k_F \). The result is

\[ (a) \propto mV^2|\pi^2/3 - (|P + I|)/k_F \ln((|P + I|)/k_F) - 2(P + I)/k_F + O(P^2, I^2)| \]

at \( k = k_F + sP + sI \) and \( I \leftrightarrow -I \) in (17) near the other
Fermi point \( k = -k_F - sP + sI \). The infinite slope seen in equation (17) at \( J = P = 0 \) (by virtue of \( \delta \) and \( \delta \)) results in logarithmically diverging second order contributions to \( v_{\uparrow \sigma} - v_{\uparrow} \) and to \( v_{\downarrow \sigma} - v_{\downarrow} \) as a function of \( P \) or \( J \) which dominate over the non-diverging HF-term \( c \). The LA comprises in summing the leading logarithmically diverging contributions to the spin velocity which is one reason for its success regarding spin sector properties. A finite interaction range does not remove logarithmic divergencies to qualitatively alter this observation.

V. OUTLOOK

In conclusion, we have generalized the ladder approximation (LA) to investigate the spin sector of single channel quantum wires in the presence of a realistic microscopic interaction. While the numerical effort is considerably smaller, we obtain values for the spin velocities that compare well with existing quantum Monte-Carlo data at not too small particle densities. The LA accounts for interaction diagrams which renormalize the spin conductance. Furthermore, the LA diagrams include the leading logarithmically diverging contributions to spin conductance and susceptibility and thus are of dominant importance for magnetic properties. The self-consistent Hartree-Fock approximation (HF) misses these diagrams and therefore leaves the spin conductance unaffected by interactions leading to an erroneous result for the spin velocity. The short distance part of the interaction is identified to govern spin sector properties. Metal gates fabricated close to a quantum wire will screen the long range part of the interaction but leave spin properties almost unaffected.

The LA should prove useful to study spin properties of multi-channel quantum wires where the numerically exact methods would be even more demanding than already in the single channel case. Compared to the HF the LA does not suffer from incommensurate densities \( k_F \neq k_F \) at finite magnetizations. This advantage over the HF might even carry over to the charge sector of coupled quantum channels since it is likely that incommensurate particle densities in different channels will cause similar instabilities of the HF-procedure as for magnetic properties in single channels. Thus, the LA might prove as the method of choice also for the charge sector of multi-channel quantum wires.

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