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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 nontrivial 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,^{1,2} in contrast to the Fermi liquids of higher dimensionality.³ Theoretical considerations based on the Tomonaga-Luttinger liquid⁴ (TLL) have predicted this behavior¹ and recent experiment^{5,6} has provided strong evidence supporting different velocities v_ρ and v_σ . 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_σ is decisive to predict spin transport^{8,9} and magnetic properties.¹⁰ Within the random phase approximation (RPA), or when treating left and right going particles as distinguishable^{2,11} as originally done by Luttinger,⁴ $v_\sigma = v_F$ stays unrenormalized with interactions.¹² 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_σ/v_F decreases with increasing interparticle repulsion in quantum wires,¹³ in qualitative resemblance to the Hubbard model.⁷ Values of $v_\sigma/v_F \approx 0.5$ have been estimated¹³ for present day single channel quantum wires.¹⁴⁻¹⁶

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 have been investigated. A future study of multichannel 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 (HF) approximation has proven as useful to estimate boundary exponents¹⁷ and, when carried out self-consistently, to yield amazingly quantitative results in charge sector;¹⁸ it captures for example very well the nonmonotonous dependence of K_ρ 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.¹⁹ 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 matter²⁰ but it performs remarkably well for the also strongly correlated charge sector of a 1DES.^{21,22}

In comparison to other Fermi-liquid methods,²² such as the Singwi, Tosi, Land, and Sölander (STLS) approximation scheme,²³⁻²⁵ the LA is known to account well for short distance properties of the interaction when tested²³ with exactly solvable models.²⁵ 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 nonzero magnetizations and for spin currents to gain homogeneous and static spin susceptibilities. Summing ladder diagrams yields estimates to v_σ that compare well with existing QMC data at not too low electron densities while the numerical effort stays comparable to self-consistent HF calculations. This enables us to scan different parameters of the microscopic interaction. 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 use¹⁹

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

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 interaction 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 subbands starts. We do not consider this case here.

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

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

$c_{k,s}$ 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 (2) 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 renormalization group (RG) method in course of which they would renormalize all prefactors of the quadratic terms, i.e., the TLL velocities $v_{N\nu}$ and $v_{J\nu}$ in

$$H_{\text{TLL}} = \sum_{\nu=\sigma,\rho} v_\nu \sum_{q \neq 0} h_{\nu,q} + \frac{\pi}{4L} \sum_{\nu=\sigma,\rho} (v_{N\nu} N_\nu^2 + v_{J\nu} J_\nu^2). \quad (3)$$

In practice such a RG approach to the quantitative values of the TLL parameters has not been tested and seems not promising for strong interactions. On the other hand, there is little doubt that the 1D electron liquid remains in the TLL phase even at strongest interactions. Fortunately, exact thermodynamic relations allow quantitative determination of the TLL velocities $v_{N\nu}$ and $v_{J\nu}$, related with the total charge or spin N_ν and the total currents J_ν , from homogeneous and static susceptibilities since the latter are observable quantities.

Symmetries reduce the number of independent TLL parameters to be determined for given microscopic single-particle dispersion $\epsilon(k)$ and interaction $V(q)$. Left-right symmetry, $\epsilon(k) = \epsilon(-k)$ leads to the TLL relations

$$v_\nu^2 = v_{N\nu} v_{J\nu} \quad (4)$$

for the sound velocities v_ν at which bosonic charge or spin-density fluctuations move, as described by the operators $h_{\nu,q}$ in Eq. (3). Most quantum wires, furthermore, show Galilei invariance in charge sector which leads to $v_{J\rho} = v_F$, indepen-

dent of the interaction. Spin rotation SU(2) invariance, present in Eq. (2) without a Zeeman field or spin-orbit coupling,⁹ ensures the three velocities $v_\sigma = v_{N\sigma} = v_{J\sigma}$ to be equal in spin sector.¹⁰

Here we concentrate on spin sector, where the thermodynamic relations read (see, e.g., Ref. 10)

$$v_{N\sigma} = \frac{2}{\pi\chi} = \frac{2L\partial^2 E_0}{\pi\partial N_\sigma^2} = \frac{\pi}{2} \frac{\partial^2 E_0/L}{\partial P^2},$$

and

$$v_{J\sigma} = \frac{2L\partial^2 E_0}{\pi\partial J_\sigma^2} = \frac{\pi}{2} \frac{\partial^2 E_0/L}{\partial I^2}. \quad (5)$$

$P = \pi N_\sigma/2L$ and $I = \pi J_\sigma/2L$ represent magnetization and spin current, respectively.

For later comparison with the HF approximation it is useful to express ground-state energies and susceptibilities in terms of the self-energy

$$\Sigma_s(k, \omega) = G_s^0(k, \omega)^{-1} - G_s(k, \omega)^{-1}. \quad (6)$$

$G_s(k, \omega)$ is the full electron propagator with respect to Eq. (2) and $G_s^0(k, \omega) = (\omega - k^2/2m + \text{sgn}[(k-sI)^2 - (k_F + sP)^2]i0)^{-1}$ the free propagator. The ground-state energy, required in Eq. (5), can be expressed as²⁶

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

which reduces to

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

for self-energies not depending on frequency ω (and therefore are real as a consequence of the Lehmann representation of G_s). This condition is fulfilled within the HF (cf. Eq. (13) 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^{11,27} of the boson model (3).

It can serve as a test to the quality of any approximative scheme in spin sector whether or not it respects the condition¹⁰ $v_{N\sigma} = v_{J\sigma}$ dictated by SU(2) invariance. The HF, for example, leaves $v_{J\sigma} = v_F$ independent of interactions since it ignores $2k_F$ interactions between electrons of opposite spins and thus violates spin rotation symmetry. The STLS only allows to calculate magnetic susceptibilities $v_{N\sigma}$ in spin sector,²⁸ 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 $v_{N\sigma}$ compared to v_F . 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.

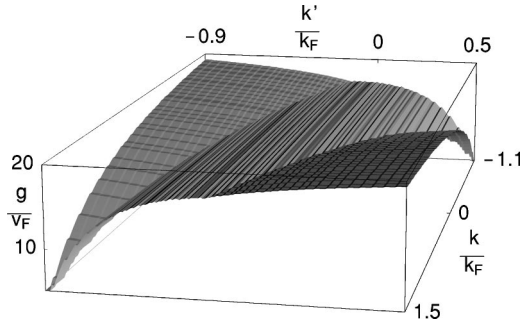


FIG. 1. Self-consistent $g_{\uparrow\downarrow}(k, k', 0)$ for $R/d = 14.14$, $k_F d = 0.15$, $P = 0.3$, $I = 0.2$. Due to correlation effects the Brueckner interaction vertex shows pronounced valleys along $k + k' = \pm 2P$. The bare value $V(0) = 22.29v_F$.

II. LADDER APPROXIMATION

To introduce the LA we follow the Refs. 26 and 21 but generalize the calculations for finite magnetization P and spin current I . The self-energy shift

$$\Sigma_s(k; P, I, k_F) = \frac{1}{2\pi} \sum_{s'} \int_{-k_F + s'(I-P)}^{k_F + s'(I+P)} dk' [g_{ss'}(k, k', 0) - \delta_{ss'} g_{ss'}(k, k', k - k')] \quad (9)$$

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 Eq. (8) and, by virtue of Eq. (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 1D electron liquids.^{21,29}

For the ladder approximation a Bethe-Salpeter integral equation

$$g_{ss'}(k, k', q) = V(q) + \frac{1}{2\pi} \int_{-\infty}^{\infty} dp g_{ss'}(k, k', p) \times K_{ss'}(k, k', p) V(q - p) \quad (10)$$

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

$$K_{ss'}(k, k', p) = 2m \frac{\Theta(|k - sI - p| - k_{Fs}) \Theta(|k' - s'I + p| - k_{Fs'})}{k^2 + k'^2 - (k - p)^2 - (k' + p)^2}. \quad (11)$$

In Eq. (11) we have defined spin dependent Fermi momenta $k_{Fs} \equiv k_F + sP$ at finite magnetizations. We solve Eq. (10) for each pair of momenta (k, k') and spins (s, s') the Householder method after mapping the infinite p 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 $g \sim N^{-2}$ due to the cusps of $g(k, k', q)$ at $q = 2k_F$]. Only at

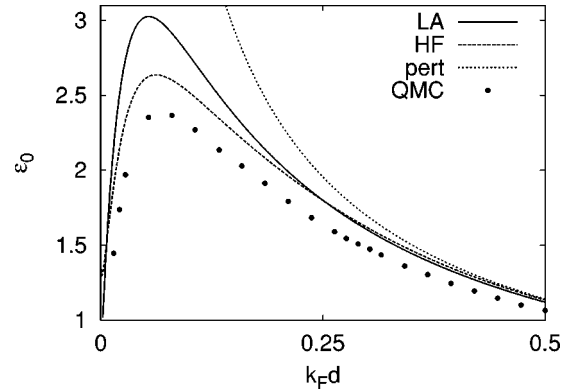


FIG. 2. Ground-state energy $\varepsilon_0 = E_0 / (Lk_F^3/m)$ vs $k_F d$ for $R/d = 14.14$. The electron density $2k_F/\pi$ can be expressed through the electron gas parameter $r_s = \pi/(8k_F a_B)$ at $d = a_B/2$. “LA” are our results, pert denotes first-order perturbation theory when $g(k, k', q) \equiv V(q)$. “HF” refers to self-consistent Hartree-Fock results of Ref. 19 and the QMC data are taken from Ref. 13.

strong interactions, when spin velocities drop below half of the Fermi velocity, we used $N = 250$. Finally, ground-state energies are integrated via Eqs. (8) and (9) 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. Fig. 1, arising primarily from the short distance correlations at $k = -k'$. Ignoring this dependence, as it is commonly done in 3D (cf. Ref. 29 and references therein), would clearly not be justified. This correlation has similarities to the striking antiferromagnetic $2k_F$ modulations found in the self-consistent HF density in 1D (Ref. 19) 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 data¹³ can be regarded as exact within symbol size. Remarkably, at densities $k_F d \gtrsim 0.2$,

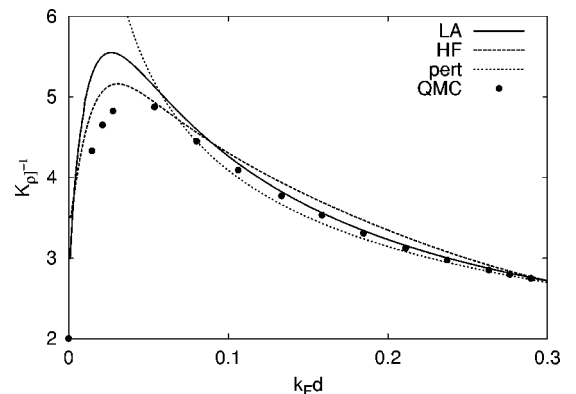


FIG. 3. Charge sector Luttinger parameter K_ρ vs $k_F d$ for $R/d = 14.14$. Labels as in Fig. 2.

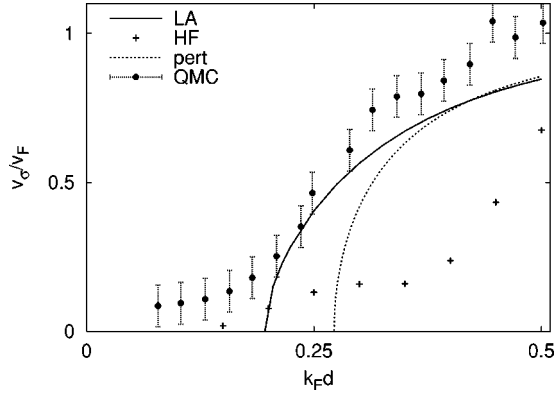


FIG. 4. Spin velocities in units of v_F vs $k_F d$ for $R/d=14.14$. The HF data are taken from Ref. 19 and the QMC data from Ref. 13.

where self-consistence 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 Fig. 3 the LA also yields better values of K_ρ in this regime. Only at smaller electron densities HF theory engenders lower ground-state energies and a better estimate to the K_ρ parameter ($k_F d < 0.1$). This energy gain is accompanied by spontaneous symmetry breaking and pronounced (though unreal) static $4k_F$ periodic Wigner crystal-like modulations¹⁹ 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 sector¹⁹ as seen in Fig. 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_σ^{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 fillings³⁰ to which quantum wires should cross over¹⁹ when the interparticle 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 .^{19,31} This is consistent with the perturbative result according to which $V(k=2k_F)$ but not $V(k=0)$ governs the magnetic susceptibility where

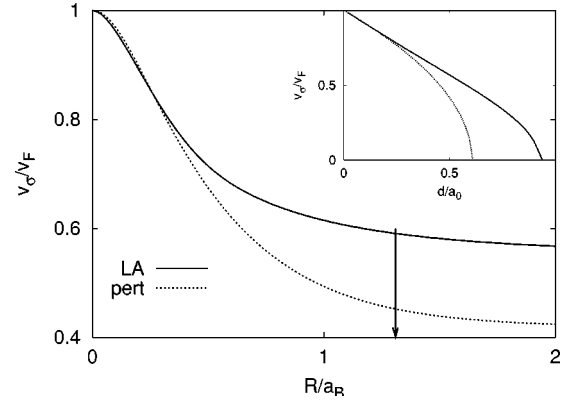


FIG. 5. Spin velocity vs interaction range R for $k_F d=0.3$. At the arrow $R = \pi/4k_F = 2r_s a_B$. When $R \ll d$ the interaction (1) vanishes trivially; we always assume $R \gg d$. The inset shows spin velocity vs wire width d at fixed $k_F d=0.3$ at $R/d=14.14$.

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 nanotubes³² where $k_F R$ can be of the order of 10^3 . The inset of Fig. 5 complements Fig. 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 LA and HF approximations to the self-energy (6), respectively, expanding it to second order in the interaction. The first-order contribution, obtained by putting $g(k, k', q) = V(q)$ in Eq. (9), yields

$$\Sigma_{s,\text{pert}}(k+sI) = \frac{4k_F}{2\pi} V(0) - \int_{-k_F-sP}^{k_F+sP} dk' \frac{V(k-k')}{2\pi}. \quad (12)$$

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

Self-consistent HF is described by

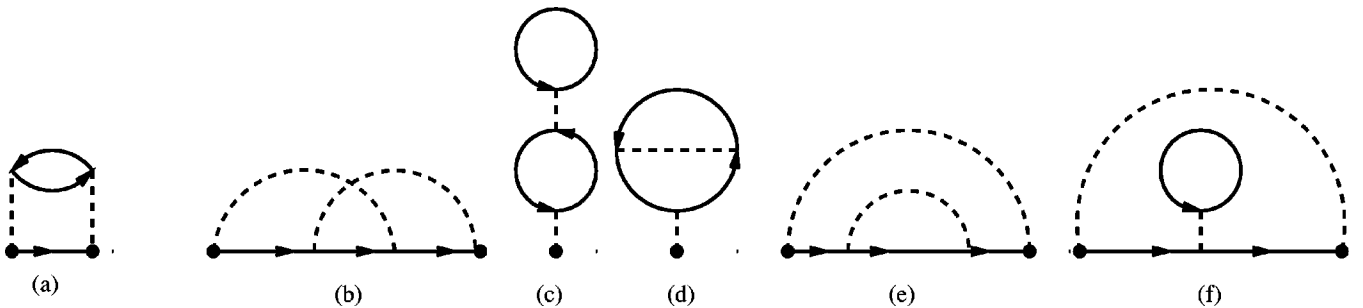


FIG. 6. Irreducible electron self-energy $\Sigma(k)$ in second-order perturbation theory. The LA accounts for the contributions (a) and (b) while the HF includes the terms (c)–(e). At $k=k_F$ the term (a) behaves like $P \ln P$ yielding a divergent contribution to v_σ .

$$\begin{aligned}\Sigma_{s,\text{HF}}(k) &= \frac{-i}{4\pi^2} \sum_{s'} \int dk' d\omega \\ &\times [V(0) - \delta_{ss'} V(k-k')] G_{s'}(k', \omega), \quad (13) \\ G_s(k, \omega) &= G_s^0(k, \omega) + G_s^0(k, \omega) \Sigma_{s,\text{HF}}(k) G_s(k, \omega). \quad (14)\end{aligned}$$

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

Second-order contributions are obtained after iterating Eqs. (9) and (10) for the LA or Eqs. (13) and (14) for the HF, respectively. For the LA this yields

$$\begin{aligned}\Sigma_{s,\text{LA}}^{(2)}(k) - \Sigma_{s,\text{pert}}(k) &= (a) + \frac{1}{(2\pi)^4} \sum_{s'} \int dk' d\omega G_s^0(k', \omega) \int dp d\omega' V(p)^2 G_s^0(k-p, k'^2/2m - \omega') G_s^0(k'+p, k'^2/2m + \omega') \\ &\quad (b) - \frac{1}{(2\pi)^4} \int dk' d\omega G_s^0(k', \omega) \int dp d\omega' V(p) V(k-k'-p) G_s^0(k-p, k'^2/2m - \omega') G_s^0(k'+p, k'^2/2m + \omega') \quad (15)\end{aligned}$$

while for the HF

$$\begin{aligned}\Sigma_{s,\text{HF}}^{(2)}(k) - \Sigma_{s,\text{pert}}(k) &= (c) - \frac{1}{(2\pi)^4} V(0)^2 \sum_{s', s''} \int dk' d\omega G_{s'}^0(k', \omega) \int dp d\omega' G_{s''}^0(p, \omega')^2 \\ &\quad (d) + \frac{1}{(2\pi)^4} V(0) \sum_{s'} \int dk' d\omega G_{s'}^0(k', \omega) \int dp d\omega' V(k'-p) G_{s'}^0(p, \omega')^2 \\ &\quad (e) - \frac{1}{(2\pi)^4} \int dk' d\omega G_s^0(k', \omega) \int dp d\omega' V(k-p) V(p-k') G_s^0(p, \omega')^2 \\ &\quad (f) + \frac{1}{(2\pi)^4} V(0) \sum_{s'} \int dk' d\omega G_{s'}^0(k', \omega) \int dp d\omega' V(k-p) G_s^0(p, \omega')^2. \quad (16)\end{aligned}$$

These are all irreducible second-order contributions. None of the diagrams, depicted in Fig. 6, occurs in both of the approximations, insofar the LA and the HF can be regarded as complementary. It is known¹¹ that any finite (but the first) order self-energy contribution diverges logarithmically for $k \rightarrow k_F$; to second order this occurs only due to the “LA terms” (a) and (b) while the HF contributions remain finite.

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

In order to compare the importance of the different terms (a)–(f) regarding $\partial_P \Sigma_s^{(2)}(k; P, I, k_F)$ and thus the magnetic susceptibility $v_{N\sigma}$ 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 nonvanishing. The latter is not divergent while term (a) can be expressed by sums of dilogarithms³³ which can further be analyzed for $I, P \ll k_F$. The result is

$$\begin{aligned}(a) \propto m V^2 [\pi^2/3 - (|P+I|)/k_F \ln[(|P+I|)/k_F] \\ - 2(P+I)/k_F + O(P^2, I^2)] \quad (17)\end{aligned}$$

at $k = k_F + sP + sI$ and $I \leftrightarrow -I$ in Eq. (17) near the other Fermi point $k = -k_F - sP + sI$. The infinite slope seen in Eq. (17) at $I = P = 0$ [by virtue of Eqs. (5) and (8)] results in logarithmically diverging second-order contributions to $v_{J\sigma} - v_F$ and to $v_{N\sigma} - v_F$ as a function of P or I which dominate over the nondiverging 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 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 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 multichannel 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 $k_{F\uparrow} \neq k_{F\downarrow}$ 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.¹⁹ Thus, the LA might prove as the method of choice also for the charge sector of multichannel quantum wires.

ACKNOWLEDGMENTS

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