$4k_F$ response function in the Tomonaga model

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We calculate the $4k_F$ response function for a one-dimensional Fermi gas using a model containing an off-site interaction V of the Tomonaga form. The approach of Dzyaloshinskii and Larkin extended by Fogedby is employed, and the result is consistent with those of Emery and those of Lee *et al.*

I. INTRODUCTION

Recently, the experimental observation[1,2] of the $4k_F$ scattering in tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ) has aroused a great deal of interest. Although many of the other experiments on TTF-TCNQ have given results consistent with a weak coupling theory, this observation of $4k_F$ cannot satisfactorily be understood from such a theoretical framework.[3] In fact, calculations by Emery[4] and by Lee, Rice, and Klemm[5] (LRK) indicated that the $4k_F$ response can only be observed if the interactions are strong, or are at least of intermediate strength. However, if the interactions are not weak, then the Fermi surface is smeared out at k_F,[6,7] and thus the single-particle picture of interaction fermions appears to break down. Although Emery has performed a correct calculation of the $4k_F$ response function for intermediate coupling using the technique of Luther and Emery,[8] this approach has to date not been universally accepted or understood. In order to give some check on Emery's results, LRK summed the leading parquet graphs, which gave a result consistent with Emery's expanded to lowest order in the interaction strengths. However, their approach is only valid for weak-interaction strengths, and thus does not serve as a reliable check in the intermediate-coupling-strength regime. We remark that the results we expect should depend in an essential way upon the strength of the interaction, and may also depend somewhat upon the form of the interaction chosen. In order to give a check on Emery's result for intermediate-interaction strengths, we shall calculate the $4k_F$ response function in the Tomonaga model, which may be performed exactly by standard methods of many-body theory.

II. MODEL

We consider the Tomonaga Hamiltonian for electrons on a single chain with off-site interactions:

$$H = H_0 + H_1 , \tag{1}$$

where

$$H_0 = \sum_{k\sigma} (\epsilon_k - \mu) a^\dagger_{k\sigma} a_{k\sigma} \tag{2}$$

is the free-particle Hamiltonian, and

$$H_1 = \tfrac{1}{2} \sum_{ij} V_j n_i n_{i+j} \tag{3}$$

is of the off-site Hubbard form, where $a_{i\sigma}$ $(a^\dagger_{i\sigma})$ annihilates (creates) an electron, on the ith site with spin $\sigma = \pm 1$, $a_{k\sigma} = L^{-1/2} \sum_j e^{ijs} a_{j\sigma}$, where L is the length of the chain, s is the lattice spacing, μ is the Fermi level, and $n_i = \sum_\sigma a^\dagger_{i\sigma} a_{i\sigma}$ is the total number operator for electrons on site i. In Eq. (3), V_j is assumed to be slowly varying with j, and the long-range part of the interaction is presumed to be the most important.

Equation (3) may be written in Fourier space as

$$H_1 = \frac{1}{2L} \sum_k V_k \rho_k \rho_{-k} , \tag{4}$$

where

$$\rho_k = \frac{1}{\sqrt{L}} \sum_j n_j e^{ijk} . \tag{5}$$

Since we are interested only in the long-range part of H_1, the sum over k in Eq. (5) may be restricted to $|k| \leq \Lambda$, where the cutoff $\Lambda \ll k_F$, and k is measured relative to k_F.

III. $4k_F$ RESPONSE FUNCTION

Since we consider only excitations near the Fermi surface, the free-particle spectrum may be linearized, and we may obtain

$$H_0 = v_F \sum_{ks} k (a^\dagger_{1ks} a_{1ks} - a^\dagger_{2ks} a_{2ks}) \tag{6}$$

and

$$H_1=\frac{1}{2L}\sum_k \{V_1[\rho_1(k)\rho_1(-k)+\rho_2(-k)\rho_2(k)] + V_2(\rho_1(k)\rho_2(-k)+\rho_2(k)\rho_2(-k)]\}, \tag{7}$$

where the indices 1 and 2 refer to different sides of the Fermi "surface," and where we have allowed the interactions between electrons on the same side (V_1) and on opposite sides (V_2) of the Fermi surface to be different for generality, but Eq. (4) has $V_1=V_2=V_{k=0}=\sum_j V_j$.

We now wish to calculate the $4k_F$ response function. Emery[4] argued that the $4k_F$ response could arise in second order from an electron-phonon interaction involving two electrons. Thus the appropriate response for small U is a linear response to the four-body operator

$$\mathcal{O}(xt)\equiv\psi_{1\uparrow}(xt)\psi_{1\downarrow}(xt)\psi^\dagger_{2\downarrow}(xt)\psi^\dagger_{2\uparrow}(xt),$$

where $\psi_{i\uparrow}(xt)$ $[\psi^\dagger_{i\downarrow}(xt)]$ annihilates (creates) an electron on the $i=1,2$ branch with spin up (down) at position x and time t. Therefore the linear $4k_F$ response may be written[4,5]

$$\chi_{4k_F}(12)=\frac{\langle 0|Te^{-i\rho V\rho/2}\mathcal{O}(1)\mathcal{O}^\dagger(2)|0\rangle}{\langle 0|e^{-i\rho V\rho/2}|0\rangle}, \tag{8}$$

where T is the time-ordering operator, 1 and 2 refer to different positions and times, and we have used the matrix notation analogous to that of Fogedby[9] for H_1,

$$V\equiv\begin{pmatrix} V_1 & V_2 \\ V_2 & V_1\end{pmatrix} \tag{9}$$

and it is understood that we integrate over momentum and time in $\rho V\rho$. Following Fogedby,[9] who extended the work of Dzyaloshinskii and Larkin[10] to calculate the two-body correlations functions, we write

$$\chi_{4k_F}=\frac{\langle b|e^{ibVb/2}\overline{Z}_1\overline{Z}_2\overline{P}_1(12)\overline{P}_2(21)|b\rangle}{\langle b|e^{ibVb/2}\overline{Z}_1\overline{Z}_2|b\rangle}, \tag{10}$$

where

$$\overline{Z}_i\equiv\langle 0|Te^{-i\rho_i b_i^\dagger}|0\rangle \tag{11}$$

and

$$\overline{P}_i(12)=\overline{Z}_i^{-1}\langle 0|Te^{-i\rho_i b_i^\dagger}\psi_{i\uparrow}(1)\psi_{i\downarrow}(1)\psi^\dagger_{i\downarrow}(2)\times\psi^\dagger_{i\uparrow}(2)|0\rangle, \tag{12}$$

where we have used the property[9]

$$\langle 0|Te^{i\rho M\rho}\cdots|0\rangle=\langle b|e^{-ibMb}\langle 0|Te^{-i\rho b^\dagger}\cdots|0\rangle|b\rangle, \tag{13}$$

where b is a Bose operator.

Since the spin-up operators do not interact with the spin-down operators, we have

$$\overline{P}_i(12)=\overline{G}_{i\uparrow}(12)\overline{G}_{i\downarrow}(12), \tag{14}$$

where

$$\overline{G}_{is}(12)=\overline{Z}_i^{-1}\langle 0|Te^{-i\rho_i b_i^\dagger}\psi_{is}(1)\psi^\dagger_{is}(2)|0\rangle, \tag{15}$$

where $s=\pm1$. We now note that Dyson's equation can be solved exactly[9] to give

$$\overline{G}_{is}(12)=G^0_{is}(12)\exp\left(i\int d3[G^0_{is}(13)-G^0_{is}(23)]b_i^\dagger(3)\right), \tag{16}$$

where

$$G^0_{is}(12)=\langle 0|T\psi_{is}(1)\psi^\dagger_{is}(2)|0\rangle \tag{17}$$

is the noninteracting single-particle Green's function for an electron moving in the ith direction with spin s. The partition function $\overline{Z}_i$ may be written as

$$\overline{Z}_i=\exp\left(-\tfrac{1}{2}\int d1\,d2\,b_i^\dagger(1)\pi_i^0(12)b_i^\dagger(2)\right), \tag{18}$$

where

$$\pi_i^0(12)=\tfrac{1}{2}\sum_s\langle 0|T\rho_{is}(1)\rho_{is}(2)|0\rangle \tag{19}$$

is the unperturbed polarization function. Writing

$$\pi\equiv\begin{pmatrix}\pi_1^0 & 0\\ 0 & \pi_2^0\end{pmatrix}, \tag{20}$$

$$K(12)\equiv\begin{pmatrix}K_1(12) & 0\\ 0 & -K_2(12)\end{pmatrix}, \tag{21}$$

where

$$K_i(12)b_i^\dagger=\sum_s[G^0_{is}(13)-G^0_{is}(23)]b_i^\dagger(3) \tag{22}$$

and repeated indices are integrated over, we may write the $4k_F$ response function

$$\chi_{4k_F}=G^0_{1\uparrow}(12)G^0_{1\downarrow}(12)G^0_{2\uparrow}(21)G^0_{2\downarrow}(21)\times\frac{\langle b|\exp[\frac{1}{2}ibVb+\frac{1}{2}b^\dagger(-\pi)b^\dagger+iK(12)b^\dagger]|b\rangle}{\langle b|\exp[\frac{1}{2}ibVb+\frac{1}{2}b^\dagger(-\pi)b^\dagger]|b\rangle}. \tag{23}$$

We observe that Eq. (23) is remarkably similar to the analogous equation for the $2k_F$ response function, differing only by a factor of 2 in the K matrices due to both up and down spins, and there are four unperturbed Green's functions instead of two.

Since both spin directions are included in a symmetric fashion, the spin degrees of freedom do not enter explicitly into our final result for χ_{4k_F}. Thus the $4k_F$ susceptibility can be thought of entirely as a charge-density wave, unlike the $2k_F$ "charge-density-wave" response function, which depends on both charge- and spin-density degrees of freedom.

The matrix element in Eq. (23) may be readily evaluated[9] to give

$$\chi_{4k_F}(12) = G_1^{02}(12)G_2^{02}(12)e^{-iK(12)DK(12)/2}, \tag{24}$$

where

$$D \equiv -i[\pi + (iV)^{-1}]^{-1} \tag{25}$$

is given in Fourier space by

$$D(k\omega) = \frac{\omega^2 - k^2}{\omega^2 - v^2k^2}\begin{pmatrix} V_1\dfrac{\omega + wk}{\omega + k} & V_2 \\ V_2 & V_1\dfrac{\omega - wk}{\omega - k}\end{pmatrix} \tag{26}$$

where

$$v = [(1 + \tilde{V}_1)^2 - \tilde{V}_2^2]^{1/2}, \tag{27}$$

$$w = 1 + (\tilde{V}_1^2 - \tilde{V}_2^2)/\tilde{V}_1, \tag{28}$$

$\tilde{V}_i = V_i/\pi$, and we have set $v_F = 1$. For k, $\omega \ll \Lambda$, we therefore obtain

$$\ln\left(\frac{\chi_{4k_F}(k\omega)}{G_1^{02}G_2^{02}}\right) = 8\pi i\left(\frac{1 + \tilde{V}_1 - \tilde{V}_2}{v}\,\frac{v}{\omega^2 - v^2k^2} - \frac{1}{\omega^2 - k^2}\right). \tag{29}$$

Taking the Fourier transform, we obtain the following behavior for x, $vt \gg \Lambda$:

$$\chi_{4k_F}(xt) = (x^2 - v^2t^2)^{-2\gamma}, \tag{30}$$

where

$$\gamma = \left(\frac{1 + \tilde{V}_1 - \tilde{V}_2}{1 + \tilde{V}_1 + \tilde{V}_2}\right)^{1/2}. \tag{31}$$

Thus, for $q \simeq 4k_F$, the $4k_F$ response behaves as

$$\chi_{4k_F}(\omega) \sim \omega^{-2+4\gamma} \tag{32}$$

for $\omega \ll \Lambda$.

We note that Eq. (32) is consistent with the result of Emery[4] if we set $\tilde{V}_1 = 0$ and $\tilde{V}_2 = \tilde{V} - \frac{1}{2}\tilde{U}_{\parallel}$ in his notation. The quantity $\tilde{V}_1$ is equivalent to $\tilde{g}_4$ in the usual Fermi-gas notation, and we have neglected the effect of backscattering, which in Emery's calculation did not effect the $4k_F$ function in an essential way.[4] Equation (32) is also consistent with the lowest-order parquet-graph result of LRK, if we expand γ to lowest order in $\tilde{V}_2 = \tilde{g}_2$, set $\tilde{V}_1 = 0$, and neglect the backscattering in their model. Thus it appears that insofar as the backscattering can be neglected, the Luther-Emery technique of representing a fermion field by the exponential of a boson field gives the correct asymptotic behavior for the four-body as well as one- and two-body correlations functions.

We note that our approach might be extended to include parallel-spin backscattering to all orders by including bosonlike spin-density operators in H_1. The anti-parallel-spin backscattering can only be treated in perturbation theory, using this approach.

IV. CONCLUSION

We have calculated the $4k_F$ response function exactly within the Tomonaga model, without using the "bosonization" procedure employed by Emery to represent the fermion fields in terms of Bose operators. The procedure we have used is that employed by Fogedby for the two-particle response functions, and is exact for the simple model we have chosen. Although real systems also contain backscattering, an exact treatment of that problem does not as yet appear to be possible. However, from the approaches of Emery[4] and Lee, Rice, and Klemm,[5] it appears that the $4k_F$ function can only diverge for at least intermediate-strength forward scattering; we believe that the model we have considered contains most of the essential physics with regard to the question of the divergence of the $4k_F$ response function.

In a real system, there will also be additional other types of interactions, such as electron-phonon interactions and interchain coupling, which may cause the effective interaction strengths to be temperature dependent. The latter in particular give rise to an effective backscattering (or on-site) interaction that changes sign as the temperature is decreased.[5] Thus there may be a crossover from $4k_F$-dominant behavior at high temperatures to $2k_F$-dominant behavior at lower temperatures (but still above the three-dimensional transition). This picture is discussed in more detail elsewhere.[11]

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