Single-particle states, Kohn anomaly, and pairing fluctuations in one dimension

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(Received 15 October 1973)

We compute the single-particle spectral density, susceptibility near the Kohn anomaly, and pair propagator for a one-dimensional interacting-electron gas. With an attractive interaction, the pair propagator is divergent in the zero-temperature limit and the Kohn singularity is removed. For repulsive interactions, the Kohn singularity is stronger than the free-particle case and the pair propagator is finite. The low-temperature behavior of the interacting system is not consistent with the usual Ginzburg-Landau functional because the frequency, temperature, and momentum dependences are characterized by power-law behavior with the exponent dependent on the interaction strength. Similarly, the energy dependence of the single-particle spectral density obeys a power law whose exponent depends on the interaction and exhibits no quasiparticle character. Our calculations are exact for the Luttinger or Tomonaga model of the one-dimensional interacting system.

I. INTRODUCTION

Interest in one-dimensional systems has recently been regenerated, largely in response to experiments on organic complexes of predominantly one-dimensional electronic character.[1,2] Some of these experiments are interpreted as providing evidence for the Peierls instability,[3] and a theory for understanding the one-dimensional fluctuations near such an instability has been proposed.[4] It has also been suggested that the dramatic increase in conductivity reported for the tetrathiofulvalinium-tetracyanoquinodimethan (TTF-TCNQ) system[1] could be caused by one-dimensional fluctuations of a superconducting order parameter.[5]

These interpretations are based, at least implicitly, on a picture of one-dimensional electronic states for which the electron-electron interaction causes no qualitative changes to the single-particle states beyond simple renormalizations. Since the work of Mattis and Lieb,[6] however, it has been known that the usual quasiparticle picture does not apply to one-dimensional interacting systems. Conventional perturbation or fluctuation theories are therefore not obviously meaningful. We attempt here an understanding of this difficulty by calculating the single-particle Green's function $G(q,\omega)$, the particle-hole susceptibility $\chi(q,\omega)$ near the Kohn anomaly, and the pair propagator $P(q,\omega)$.

The character of the superconducting fluctuations are described by P, and it is an obvious response function to study. From G, the spectral weight of the single-particle excitations is determined, and the importance of interactions in causing departures from the quasiparticle picture directly evaluated. From $\chi(q,\omega)$ at momenta near twice the Fermi momentum $q\simeq 2k_F$, the low-lying excitations of the interacting-electron gas are computed and the modification of the Peierls instability due to interactions is discussed. Our calculations for G, χ, and P are exact within the Luttinger or Tomonaga model of the interacting-electron gas.

In order to compute these functions, it is necessary to go beyond previous considerations of such one-dimensional systems, because the time evolution of the single-fermion operators is required. It is, in general, extremely complicated to work directly with these operators. We circumvent this difficulty by finding an operator in the boson space which satisfies the proper commutation and anticommutation relations and has the same expectation values as the original fermion operators. The computation of G, χ, and P is thereby reduced to a solvable boson problem.

Some of our new results could have been anticipated from the solution of Mattis and Lieb.[6] The spectral function, given by $\mathrm{Im}G(q,\omega)$, has a δ-function peak at zero temperature for free particles. With interactions present, this peak vanishes, and $\mathrm{Im}G(k_F,\omega)$ exhibits a power-law behavior extending to energies of the order of the bandwidth. The exponent of this power law depends on the interaction strength but not its sign. One expects to find no quasiparticle peak for this system since the discontinuity in the $T=0$ occupation number has vanished. The entire spectral weight must therefore be contained in the "incoherent background." In spite of this power law, the specific heat at low temperatures remains linear[6] in T.

The result for $\chi(q,\omega=0)$ is somewhat surprising. Smearing out the $T=0$ occupation number might be expected to weaken the logarithmic Kohn singularity at $2k_F$, just as thermal smearing of free particles converts this singularity to a $\ln T$ behavior. In fact, for *repulsive* interactions, a *stronger* power-law singularity is found, with the exponent of that power law dependent on the interaction strength. Attractive interactions do indeed give a finite $\chi(2k_F, 0)$ at $T=0$, but it is substantially smaller than one would guess from the smearing of the occupation number. Even for very weak interactions, the departures from the free-particle susceptibility are quite pronounced.

The $T=0$ dynamic susceptibility near $2k_F$ exhibits a threshold singularity for frequences at the edge of the continuum, reminiscent of the x-ray-threshold edge.[7] The edge singularity satisfies a power law, and is enhanced (divergent) for repulsive interactions and suppressed for attractive interactions. In both cases the exponent of the power law depends on the interaction strength. As in the x-ray problem, these singularities arise because the interactions cause a single-particle excitation to be "dressed" with an infinite number of particle-hole pairs. These pairs are just the large-wavelength boson excitations of the Luttinger or Tomonaga models[8] and conspire to drastically modify the low-lying excitations around $2k_F$.

The pair propagator $P(q, \omega)$ is found to be the same as $\chi(q-2k_F, \omega)$, provided the sign of the interaction strength is reversed. An attractive interaction thus produces a power-law divergence in $P(q=0, \omega=0)$ as the temperature is lowered, indicative of large pairing fluctuations. However, the functional dependence on ω, q, and T is not of the Ginzburg-Landau type, due to the power-law behavior mentioned above.

We find a new characteristic temperature, T_0, below which these interaction effects are important. This is estimated to be $T_0 \sim We^{-1/\gamma}$, where γ is an interaction parameter and W is the order of the bandwidth. Although it is possible that the models we discuss may be an inadequate description of some systems, we argue that the fluctuation effects calculated here will still be important for temperatures less than T_0. For this situation, our solutions provide a better starting point than those which involve the quasiparticle assumption.

II. SINGLE-PARTICLE GREEN'S FUNCTION

A. Field operators and Luttinger model

In this section, the formal computation of $G(q, \omega)$ is given. It proves to be simpler to work with the Fourier transform function $G(x, t)$, which is defined by

$$G(x,t) = -i\Theta(t)\langle[\psi_1(x,t), \psi_1^\dagger]_+\rangle , \tag{1}$$

where $\psi_1(x, t)$ is the field operator for the fermions (time evolved with the full Hamiltonian H), the subscript + indicates the anticommutator, and the angular brackets denote an average in the density matrix $e^{-\beta H}$. The Hamiltonian for the Luttinger model is

$$H = v_F \sum_k k(a_{1,k}^\dagger a_{1,k} - a_{2,k}^\dagger a_{2,k}) + \sum_p V_p \rho_1(p)\rho_2(-p) , \tag{2}$$

where sums are over the discrete indices of one-dimensional plane waves on a line of length L, $\psi_1(x) = L^{-1/2}\sum_k e^{ikx} a_{1,k}$, $\psi_2(x) = L^{-1/2}\sum_k e^{ikx} a_{2,k}$, V_p is the Fourier transform of the two-body interaction, it is assumed all states below the energy $k_F v_F$ are filled, and $k_F = mv_F$ is the Fermi momentum ($\hbar = 1$). The objects $\rho_1(p)$ and $\rho_2(p)$ are density operators, defined by

$$\begin{aligned} \rho_1(p) &= \sum_k a_{1,k+p}^\dagger a_{1,k} , \quad \rho_1(-p) = \sum_k a_{1,k}^\dagger a_{1,k+p} , \\ \rho_2(p) &= \sum_k a_{2,k+p}^\dagger a_{2,k} , \quad \rho_2(-p) = \sum_k a_{2,k}^\dagger a_{2,k+p} , \end{aligned} \tag{3a}$$

where $p > 0$. They satisfy a boson algebra,

$$\begin{aligned} &[\rho_1(-p), \rho_1(p')] = [\rho_2(p), \rho_2(-p')] = (pL/2\pi)\delta_{p,p'} , \\ &[\rho_1(p), \rho_2(p')] = 0 . \end{aligned} \tag{3b}$$

These relations, together with

$$\left[\rho_1(p), v_F \sum_k k a_{1,k}^\dagger a_{1,k}\right] = -v_F p \rho_1(p) \tag{4}$$

and the corresponding result for $\rho_2(p)$, permit the exact diagonalization of H. The transformation which effects this diagonalization is given by $e^{iS}He^{-iS} = H_D$, where $S = 2\pi i L^{-1}\sum_p p^{-1}\varphi(p)\rho_1(p)\rho_2(-p)$, and $\tanh 2\varphi(p) = -V_p(\pi v_F)^{-1}$. The reader is referred to the paper by Mattis and Lieb[6] for the details of this solution and the proof of the above statements. We consider now the extension of this solution to find $G(x, t)$.

A direct computation of the equation of motion for the operator $a_{1,k}$ shows that it couples to the operator $a_{1,k}\rho_2(p)$. The equation of motion for this new operator couples to yet more complicated operators, and one quickly obtains an infinite set of coupled operator equations. Clearly this brute-force approach is extremely awkward, if not impossible.

Such difficulties can be circumvented by using a new operator $O_1(x)$, which has the same equation of motion as the field operator, $\psi_1(x)$, and the same commutation relation with the density operators. This operator is defined by

$$O_1(x) = (2\pi\alpha)^{-1/2} e^{ik_F x + \phi_1(x)} , \tag{5}$$

where

$$\phi_1(x) = 2\pi L^{-1} \sum_{k>0} k^{-1} e^{-\alpha k/2}[\rho_1(-k)e^{ikx} - \rho_1(k)e^{-ikx}]$$

and α is a cutoff parameter which is determined below. Since $O_1(x)$ is expressed entirely in terms of density operators, it is obvious that correlation functions containing only products of $O_1(x,t)$ and its Hermitean conjugate can be evaluated, using the same transformations which diagonalize H.

It remains to be shown that these new correlation functions are equal to those defined with the original $\psi_1(x)$ fields. The commutation relations with density operators are[9]

$$[\psi_1(x), \rho_1(k)] = e^{ikx}\psi_1(x) , \tag{6a}$$

$$[O_1(x), \rho_1(k)] = e^{ikx}O_1(x) , \tag{6b}$$

and the equations of motion are

$$\frac{d}{dt}\psi_1(x,t) = -v_F\frac{d}{dx}\psi_1(x,t) - i\sum_p V_p e^{ipx}\psi_1(x,t)\rho_2(-p,t) , \tag{7a}$$

$$\frac{d}{dt}O_1(x,t) = -v_F\frac{d}{dx}O_1(x,t) - i\sum_p V_p e^{ipx}O_1(x,t)\rho_2(-p,t) - 2\pi i L^{-1}\sum_k e^{-\alpha k}O_1(x,t) . \tag{7b}$$

The last term in Eq. (7b) represents a constant energy shift, which can be removed by choosing a new zero of energy. Since this reference energy is irrelevant for the computation of $G(q,\omega)$, we simply discard it.

The transformation e^{iS}, which diagonalized H, involves only density operators. According to Eq. (6) $e^{iS}\psi_1(x)e^{-iS}$ will therefore transform exactly as $e^{iS}O_1(x)e^{-iS}$. The former has been evaluated previously,[6] with the result

$$e^{iS}\psi_1(x)e^{-iS} = e^{w_1(x)}e^{r_2(x)}\psi_1(x) , \tag{8a}$$

where

$$w_1(x) = 2\pi L^{-1}\sum_{k>0} k^{-1}(\cosh\varphi - 1) \times[\rho_1(-k)e^{ikx} - \rho_1(k)^{-ikx}]$$

and

$$r_2(x) = 2\pi L^{-1}\sum_{k>0} k^{-1}\sinh\varphi \times[\rho_2(-k)e^{ikx} - \rho_2(k)e^{-ikx}] .$$

The same procedure applied to the $O_1(x)$ operator gives precisely the same result

$$e^{iS}O_1(x)e^{-iS} = e^{w_1(x)}e^{r_2(x)}O_1(x) . \tag{8b}$$

Finally, consider the computation of the correlation functions $\langle G|\psi_1(x,t)\psi_1^\dagger|G\rangle$ and $\langle G|O_1(x,t)O_1^\dagger|G\rangle$ where $|G\rangle$ is the ground state of H. Let $|0\rangle$ be the ground state of H_D, which is related to $|G\rangle$ by $|G\rangle = e^{-iS}|0\rangle$. Using $e^{iS}He^{-iS} = H_D$, the correlation functions can be written

$$\langle G|\psi_1(x,t)\psi_1^\dagger|G\rangle = \langle 0|e^{iH_Dt}e^{iS}\psi_1(x)e^{-iS}e^{-iH_Dt}e^{iS}\psi_1^\dagger e^{-iS}|0\rangle , \tag{9}$$

with an identical equation for $\langle G|O_1(x,t)O_1^\dagger|G\rangle$. The relations established by Eqs. (6)–(8) ensure the equality $\langle G|\psi_1(x,t)\psi_1^\dagger|G\rangle = \langle G|O_1(x,t)O_1^\dagger|G\rangle$, provided that $\langle 0|\psi_1(x)\psi_1^\dagger|0\rangle = \langle 0|O_1(x)O_1^\dagger|0\rangle$. As shown in Ref. 6, $|0\rangle$ is just the filled Fermi sea with no boson excitations present, so that the evaluation of these latter expectation values is trivial,[10] giving (at $T=0$)

$$\langle 0|\psi_1(x)\psi_1^\dagger|0\rangle = L^{-1}\sum_{k>k_F} e^{ikx} , \tag{10a}$$

$$\langle 0|O_1(x)O_1^\dagger|0\rangle = (2\pi\alpha)^{-1}e^{ik_Fx}\exp 2\pi L^{-1}\sum_{k>0}k^{-1}e^{-\alpha k}(e^{ikx}-1) = (2\pi)^{-1}(\alpha - ix)^{-1}e^{ik_Fx} . \tag{10b}$$

In Eq. (10b), we have taken the limit $\sum_k \to L(2\pi)^{-1}\int dk$. If an infinitesimal imaginary part is added to k in Eq. (10a), to ensure convergence for large k, we have agreement provided the limit $\alpha \to 0$ is taken. The correlation functions $\langle G|\psi_1(x,t)\psi_1^\dagger|G\rangle$ and $\langle G|O_1(x,t)O_1^\dagger|G\rangle$ are therefore identical, in this limit.

There is another sense in which these correlation functions are equal which helps in the computation of χ and P. If the density of states is not a constant, as in the Luttinger model, but is chosen such that $\sum_k \to L(2\pi)^{-1}\int dk e^{-\alpha|k-k_F|}$ in Eq. (10a) there is an equality between Eqs. (10a) and (10b) even for finite α. We therefore interpret α^{-1} as the bandwidth (in momentum units) and expect this quantity to appear in our calculations whenever the bandwidth or excitations far away from the Fermi surface are important.

In a formalistic sense, our solution for dynamical quantities are exact solutions of the Luttinger model only in the limit $\alpha \to 0$. Finite α corresponds to an alteration of the energy spectrum far from the Fermi surface, as is done in the Tomonaga model. However, certain properties of the Luttinger model, such as the Kohn singularity at $2k_F$, depend only on the low-lying states. Our results for these properties are thus exact, in a very real sense, despite the necessity of a cutoff. The situation is similar to the Kondo problem,[10] where infrared singularities are determined only by the low-lying states, but a cutoff at the bandwidth is needed for convergence.

These considerations are readily extended to other correlation functions and finite temperatures. In all cases relevant for this paper, replacement of $\psi_1(x)$ by $O_1(x)$ does not change the correlation functions. As is known in the Tomonaga model for the Kondo problem, this is not always the case, and proper caution must be exercised for other correlation functions.

B. Evaluation of Green's function $G(x,t)$

Applying this method to the computation of $G(x, t)$, we find, from Eqs. (1) and (5),

$$G(x, t) = -i\Theta(t)(2\pi\alpha)^{-1}e^{ik_Fx}\langle[e^{\phi_1(x,t)}, e^{-\phi_1}]_+\rangle$$
$$= -i\Theta(t)(2\pi\alpha)^{-1}e^{ik_Fx}\langle e^{iHt}e^{\phi_1(x)}e^{-iHt}e^{-\phi_1} + (t\to -t, x\to -x)\rangle \ . \quad (11)$$

Inserting the diagonalizing transformation, e^{iS} and using Eq. (8), this expression can be written

$$G(x, t) = -i\Theta(t)(2\pi\alpha)^{-1}e^{ik_Fx} \times[\langle e^{w_1(x,t)}e^{r_2(x,t)}e^{\phi_1(x,t)}e^{-\phi_1}e^{-r_2}e^{-w_1}\rangle_D + (t\to -t, x\to -x)] \ , \quad (12)$$

where the time evolution and averaging is now performed using H_D, which is *diagonal* in the density operators. Equation (12) is thus a standard form, which is readily evaluated[11] to give the result ($T = 0$)

$$G(x, t) = -i\Theta(t)(2\pi\alpha)^{-1}\exp(ik_Fx) \times \{\exp[Q_1(x, t) + Q_2(x, t)] + (t\to -t, x\to -x)\} \ ,$$

where (13)

$$Q_1(x, t) = 2\pi L^{-1}\sum_{k>0} k^{-1}(\cosh\varphi - 1 + e^{-\alpha k})^2 \times(e^{ikx-i\epsilon_kt} - 1) \ ,$$
$$Q_2(x, t) = 2\pi L^{-1}\sum_{k>0} k^{-1}(\sinh\varphi)^2(e^{-ikx-i\epsilon_kt} - 1) \ ,$$

and $\epsilon_k = v_F k \,\mathrm{sech}\varphi(k)$. In order to complete the solution, we use the identity

$$\alpha^{-1} = (\alpha - is)^{-1}e^{-2\pi L^{-1}\sum_{k>0} k^{-1}e^{-\alpha k}(e^{ikS} - 1)}$$

and take the limit $\alpha\to 0$. For the case $t = 0^+$, we find

$$G(x, 0) = (2\pi)^{-1}e^{ik_Fx}[e^{Q(x)}(x + i0)^{-1} + (x\to -x)] \ , \quad (14)$$

where

$$Q(x) = 4\pi L^{-1}\sum_{k>0} k^{-1}\sinh^2\varphi(\cos kx - 1) \ .$$

The correlation function $\langle O_1(x)O_1^\dagger\rangle$ is thus $(2\pi x)^{-1}\times e^{ik_Fx+Q(x)}$, identical to the result of Mattis and Lieb[6] for $\langle\psi_1(x)\psi_1^\dagger\rangle$.

Equation (13) is the formal solution for $G(x, t)$ for an arbitrary interaction consistent with the limitation that φ is real. The sum rule on the spectral function $1 = -\pi^{-1}\int_{-\infty}^{\infty}d\omega\,\mathrm{Im}G(q, \omega)$ for all q is a check of the equal-time anticommutator. Since our solution reproduces the exact result in that limit, it follows without computation that this sum rule is satisfied. In the following, the evaluation $G(q, \omega)$ for a special form of V_p is given. It is an approximation to Eq. (13), and therefore does not satisfy the sum rule exactly, although it does lend considerable insight into the exact structure of $G(q, \omega)$.

In order to proceed with the Fourier transformation leading to $G(q, \omega)$, it is necessary to assume a particular form for the interaction V_p. This is taken to be $\sinh^2\varphi(p) = \gamma e^{-pr}$, where r is the range of the interaction and γ can be related to $V_{p=0}$ through $\tanh 2\varphi(0) = -V_0(\pi V_F)^{-1}$. The excitation spectrum $\epsilon_p = v_F p\,\mathrm{sech}\varphi(p)$ is approximated by $\epsilon_p = cp$, where c is the renormalized Fermi velocity, $c = v_F\mathrm{sech}\varphi(0)$. We are primarily interested in excitations near the Fermi level and their consequences; the precise details of the large momentum states are not of interest here. Results which depend on r cannot be regarded as "universal," since another form for V_p could give a different answer. However, certain features will be independent of r, and these we argue to be a general property of the system.

With this assumed V_p and ϵ_p, the integrals for $Q_1(x, t)$ and $Q_2(x, t)$, are easily evaluated, leading to the result at zero temperature:

$$G(x, t) = i\Theta(t)\pi^{-1}e^{ik_Fx} \times\mathrm{Im}\left\{(x - ct + i0)^{-1}\left[\left(\frac{x}{r}\right)^2 + \left(1 + \frac{ict}{r}\right)^2\right]^{-\gamma}\right\} . \quad (14')$$

The power-law behavior, induced by the interactions, is a "universal" feature of this model.

Fourier transforming Eq. (14′) is tedious but straightforward. Taking the imaginary part of the two terms in the curly brackets, we find $G(q, \omega) = G_1(q, \omega) + G_2(q, \omega)$, where

$$G_1(q', \omega) = -ic^{-1}\int_0^\infty dt\int_{-\infty}^\infty dx e^{i\omega t - iq'x}\delta(s) \times\mathrm{Re}[F(s)F(s')] \ ,$$
$$G_2(q', \omega) = -i(\pi c)^{-1}\int_0^\infty dt\int_{-\infty}^\infty dx\, e^{i\omega t - iq'x}s^{-1} \times\mathrm{Im}[F(s)F(s')] \ . \quad (15)$$

Here, we have defined $q' = q - k_F$, $s = t - x/c$, $s' = x/c + t$, and $F(s) = (1 + isc/r)^{-\gamma}$. The first of these can be written

$$G_1(q', \omega) = -i\left(\frac{r}{c}\right)^\gamma\int_0^\infty dt e^{i(\omega - cq')t}\mathrm{Re}\left(\frac{r}{c} + 2it\right)^{-\gamma} . \quad (16)$$

For $\omega - cq'$ sufficiently small, only the long-time behavior is important in this integral, and r/c can be neglected in comparison with t, provided $\gamma < 1$.

The integral can then be reduced to a Γ function, by changing variables, $i(\omega - cq')t \to -t'$, and rotating the contour of integration in the t' plane, so that the integral on t' runs from 0 to $+\infty$. The result is

$$G_1(q',\omega) \cong \frac{\Gamma(1-\gamma)}{\omega - cq'}\left(\frac{r(\omega - cq')}{2ic}\right)^{\gamma}\cos\tfrac{1}{2}\pi\gamma\ . \quad (17)$$

For the spectral function, we require only $\mathrm{Im}G(q',\omega)$. Using the property $G_2(q',\omega)=G_2^*(-q',-\omega)$, the limits of integration over t in Eq. (15) may be extended to $-\infty$. Changing variables to s and s' the integral for $\mathrm{Im}G_2(q',\omega)$ becomes

$$\mathrm{Im}G_2(q',\omega) = -(4\pi)^{-1}\mathrm{Im}\Big[\int_{-\infty}^{\infty} ds\, s^{-1}e^{is(\omega-cq')/2}F(s) \times \int_{-\infty}^{\infty} ds'\, e^{is'(\omega+cq')/2}F(s') + (\omega\to-\omega, q'\to-q')\Big]\ . \quad (18)$$

These integrals may be evaluated in the low-energy region, using the approximation discussed above Eq. (17). The result is

$$\mathrm{Im}G_2(q',\omega) = -2(\pi\gamma)^{-1}\left(\frac{r}{c}\right)^{2\gamma}\Gamma^2(1-\gamma) \times [\mathrm{Im}(\omega - cq')^{\gamma}\mathrm{Im}(\omega - cq')^{\gamma-1} + (\omega\to-\omega, q'\to-q')]\ . \quad (19)$$

For the momentum at the Fermi surface, $q'=0$, the spectral function $-\pi^{-1}\mathrm{Im}G(0,\omega+i0)$ is given by adding Eqs. (17) and (19) with the result

$$-\pi^{-1}\mathrm{Im}G(0,\omega+i0) \cong \frac{r}{c}\left(\frac{\omega r}{2c}\right)^{\gamma-1}\Gamma(1-\gamma)\sin\tfrac{1}{2}\pi\gamma + \left(\frac{2r}{\gamma c}\right)\left(\frac{\omega r}{2c}\right)^{2\gamma-1} \times [\Gamma(1-\gamma)\sin\pi\gamma]^2\ . \quad (20)$$

This holds for $\omega \ll c/r$, i.e., for energies much less than that corresponding to the range of the two-body force. In the opposite limit, the spectral function behaves as ω^{-2}, as can be seen directly from Eqs. (16) and (18).

This result has an interesting interpretation. The quasiparticle picture would lead to a spectral function of the form $-\pi^{-1}\mathrm{Im}G(0,\omega+i0)=Z\delta(\omega)+b(\omega)$, where Z is a single-particle residue and $b(\omega)$ is the incoherent background, whose integrated strength is $(1-Z)$. Equation (20) does not contain the δ-function and evidently $Z=0$.

It is interesting to consider the difficulties which occur if $G(q,\omega)$ is studied using perturbation theory. Leading divergences of the form $\gamma(\gamma\ln\omega)^n$ are encountered, along with other combinations of γ and $\ln\omega$. Partial summations, of the type often applied to such divergent series, might be expected to remove these singularities, replacing divergent quantities such as $\gamma^2\ln\omega$ by $\gamma^2\ln(\omega^2+c')$, where c' is some constant. Such partial summations would be highly misleading here, and we believe our result should serve as a warning for the qualitatively different effects of fluctuations in one-dimensional interacting systems.

III. SUSCEPTIBILITY OF LUTTINGER AND TOMONAGA MODELS

As discussed by many authors, the susceptibility of the one-dimensional free-electron gas diverges at twice the Fermi momentum, as the temperature is lowered to zero. The divergence is caused by transitions between states at opposite ends of the Fermi line and is properly classified as an infrared singularity. In mean-field theories, this behavior is responsible for the Peierls lattice instability, in which a phonon frequency vanishes according to the perturbation equation

$$\omega_q^2 = \omega_{0,q}^2 - \omega_{0,q}g_L^2\chi(q,\omega)\ , \quad (21)$$

where $\omega_{0,q}$ is the "unperturbed" phonon frequency and g_L the coupling constant. This soft-mode instability is therefore intimately connected with a large susceptibility.

Section II implies that departures from the free-particle result for χ might be significant, even in the absence of electron-lattice coupling. In order to understand these modifications, we study χ for the interacting gas, without coupling to the phonons. In the concluding section (Sec. IV) some possible modifications which occur when the electron-phonon coupling is introduced are briefly mentioned.

The first problem to consider is the proper definition of χ for these one-dimensional models. In the Luttinger model, the density operator which causes transitions across the Fermi line is defined by $\sigma(q)=\sum_k a_{1,k+q}^\dagger a_{2,k}$. There are additional excitations in this model, arising from transitions within the 1 or 2 branches, which are given by the usual density operators $\rho_1(q)$ and $\rho_2(q)$. The susceptibilities corresponding to these excitations have already been calculated,[6] and are approximately constant near $q=2k_F$, with no dramatic frequency, momentum, or temperature dependence. We will therefore neglect these processes here, and concentrate entirely on that susceptibility exhibiting the infrared singularity, defined by

$$\chi(x,t) = -i\Theta(t)\langle[\sigma(x,t),\sigma^\dagger]\rangle\ , \quad (22)$$

where $\sigma(x)=L^{-1}\sum_q\sigma(q)e^{iqx}=\psi_1^\dagger(x)\psi_2(x)$ and time evolution, as well as thermal averaging, is with the full H of Eq. (2).

The computation of χ can be readily performed, using the operator $O_1(x)$ [Eq. (5)] for $\psi_1(x)$, and the corresponding operator $O_2(x)=(2\pi\alpha)^{-1/2}e^{-ik_Fx+\phi_2(x)}$, where

$$\phi_2(x) = 2\pi L^{-1}\sum_{k>0} k^{-1}e^{-\alpha k/2}[\rho_2(-k)e^{ikx} - \rho_2(k)e^{-ikx}]$$

for $\psi_2(x)$. After some lengthy, but straightforward manipulations,[10] the following result is found:

$$\chi(x,t) = -i\Theta(t)(2\pi\alpha)^{-2}\exp(2ik_Fx) \times [\exp[U(x,t)+U(x,-t)] - (x\to -x, t\to -t)], \quad (23)$$

where

$$U(x,t) = 2\pi L^{-1}\sum_k k^{-1}U_k^2[n_k(e^{-ikx+i\epsilon_k t}-1) + (1+n_k)(e^{-ikx-i\epsilon_k t}-1)],$$

$n_k=(e^{\epsilon_k/T}-1)^{-1}$, and $U_k=e^{-\alpha k}+\cosh\varphi+\sinh\varphi-1$. In order to proceed further, information about the momentum dependence of U_k^2 or V_k is necessary. A convenient form for our purposes is $U_k^2=e^{-2\alpha k} - ge^{-kr}$, where r is the range and g is a measure and has the sign of the $k=0$ potential strength. The spectrum is taken to be linear, $\epsilon_k=ck$. It should be noted that this form for U_k^2 implies a slightly different V_k than was used in Sec. II.

It is also necessary to specify a density of states, because in the limit $\alpha\to 0$, $e^{U(x,t)}$ diverges at short distance and time. Those short distance singularities reflect very large momentum excitations in the Luttinger model, which do not occur in a real system with finite bandwidth. We choose a density of states corresponding to finite α, as discussed in Sec. II. This choice does not affect the "universal" nature of the infrared singularity which arises from *large* x and t. For simplicity, we take $2\alpha=r$. All of these specilizations are consistent with our focus on the contributions of the low-lying states to $\chi(q,\omega)$.

The integral for $U(x,t)$ is a standard form, which can be evaluated, giving

$$\chi(x,t) = -i\Theta(t)(2\pi\alpha)^{-2}e^{2ik_Fx}\left[\left(\frac{\Gamma(x_0-isT)\Gamma(1+x_0+isT)\Gamma(x_0-is'T)\Gamma(1+x_0+is'T)}{\Gamma^2(x_0)\Gamma^2(1+x_0)}\right)^{1-g} - (s\to -s, s'\to -s')\right], \quad (24)$$

where $x_0\equiv rT/c$, $s=t-x/c$, and $s'=t+x/c$. Using the properties of the Γ function, Eq. (24) can be simplified to

$$\chi(x,t) \cong 2(2\pi\alpha)^{-2}x_0^{2-2g}e^{2ik_Fx}\Theta(t) \times\left(\frac{\pi sT}{\sinh\pi sT}\right)^{1-g}\left(\frac{\pi s'T}{\sinh\pi s'T}\right)^{1-g} \times \mathrm{Im}(x_0-isT)^{g-1}(x_0-is'T)^{g-1}, \quad (25)$$

where the approximation indicates that x_0 has been dropped in comparison with 1. It is this form which is most convenient for the following discussion.

The Fourier transform of Eq. (25) involves a time integral from 0 to $+\infty$. Using the symmetry properties of the integrand, it is easy to show that the limits may be extended to $-\infty$ in the integral for $\mathrm{Im}\chi(q,\omega)$. The integration variables may then be changed from x and t to s and s', with the result

$$\mathrm{Im}\chi(Q,\omega) = -(4\pi^2c)^{-1}(r/c)^{-2g}[F(\omega-cQ)F(\omega+cQ) - F(-\omega+cQ)F(-\omega-cQ)], \quad (26)$$

where

$$F(z) = \int_{-\infty}^{\infty} ds\left(\frac{\pi Ts}{\sinh\pi Ts}\right)^{1-g} e^{isz/2}\left(\frac{r}{c}-is\right)^{g-1}$$

and $Q=q-2k_F$. $F(z)$ may be evaluated by making use of the approximation $\pi Ts/\sinh\pi Ts\cong e^{-\theta|s|}$, where $\theta\cong\frac{1}{2}\pi T$ is chosen to simulate the exact temperature dependence for the free gas, $g=0$. We then neglect r/c in comparison to s, which is justified provided $zr\ll c$ and $Tr\ll c$. For the case $g<0$, it is necessary to first integrate by parts before neglecting r/c, to circumvent a spurious divergence at $s=0$. The result is

$$F(z) = -2\Gamma(g)\mathrm{Im}(z/2-i\theta')^{-g}, \quad (27)$$

where $\theta'=\theta(1-g)$. This approximation is good for both positive and negative z, and $g<1$. In the zero-temperature limit, $\mathrm{Im}\chi(Q,\omega)$ is given simply by the equations

$$\begin{aligned}\mathrm{Im}\chi(Q,\omega) &= 0, \quad |\omega|<c|Q| \\ \mathrm{Im}\chi(Q,\omega) &= (\pi^2c)^{-1}(r/c)^{-2g}\Gamma^2(g)\sin^2\pi g \times[\tfrac{1}{4}(\omega^2-c^2Q^2)]^{-g}, \quad |\omega|>c|Q|.\end{aligned} \quad (28)$$

As could have been anticipated, the power-law behavior in the Green's function [Eq. (20)] has a counterpart in the susceptibility. Here, however, the sign of the potential is important—repulsive interactions ($g>0$) lead to a divergence at the edge of the continuum $\omega=\pm cQ$, while attractions cause $\mathrm{Im}\chi$ to vanish there.

The properties of $\mathrm{Re}\chi(Q,\omega)$ at $T=0$, can be understood by considering the Kramers-Kronig dispersion relation using Eq. (28). For $g>0$, the divergence at $\omega=\pm cQ$ also implies a divergence in $\mathrm{Re}\chi$ along that edge. In particular, $\mathrm{Re}\chi(Q,0)$ diverges as Q^{-2g}. A finite temperature will cause rounding of these divergences, but a peak at the edge will remain.

This dispersion integral for $\mathrm{Re}\chi(Q,\omega)$ can be evaluated, giving the result ($g>0$)

$$\mathrm{Re}\chi(Q,\omega)=(2\pi^2c)^{-1}\Gamma^2(q)\left(\frac{r}{c}\right)^{-2g}\times\mathrm{Im}\left[\left(\frac{\omega+cQ}{2}-i\theta'\right)^{-g}\times\left(\frac{\omega-cQ}{2}-i\theta'\right)^{-g}+(\omega\to-\omega)\right]. \tag{29}$$

Note the divergence of the static susceptibility at $Q=0$ is not logarithmic, but T^{-2g}, and the curvature $(\partial^2/\partial Q^2)\mathrm{Re}\chi(Q,0)|_{Q=0}$ diverges as T^{-2-2g}.

For very small g, it is necessary to modify Eq. (29) to account for the low-frequency restriction used to derive Eq. (28). This can be approximately treated with a cutoff in the dispersion integral, at $\omega\cong c/\alpha$. A correction term in Eq. (29) thereby results which is equal to $-\mathrm{Re}\chi(Q,c/\alpha)$. For example, the $T=0$ and $Q=0$ susceptibility becomes

$$\mathrm{Re}\chi(0,\omega)=(2\pi^2c)^{-1}\Gamma^2(g)\sin2\pi g\left(\frac{r}{2c}\right)^{-2g}\times\left[\omega^{-2g}-\left(\frac{c}{r}\right)^{-2g}\right], \tag{30}$$

which reduces to $2(\pi c)^{-1}\ln(c/\omega r)$ in the limit $g\to0$, the correct result for the free gas.

For attractive interactions ($g<0$), $\mathrm{Im}\chi(Q,\omega)$ vanishes as $\omega\to cQ$, therefore $\mathrm{Re}\chi(Q,\omega)$ will be finite. For large ω, Eq. (28) is proportional to $\omega^{2|g|}$, and it is thus necessary to use the cutoff procedure discussed above. The dispersion integral for the static susceptibility then gives the result

$$\mathrm{Re}\chi(Q,0)=[\pi c\Gamma^2(1+|g|)]^{-1}I(\tfrac{1}{2}Q\alpha), \tag{31}$$

where

$$I(x)=2^{-2|g|}\Gamma(2|g|,2x)+x^{2|g|}\int_1^\infty(du/u)e^{-2xu}\times[(u^2-1)^{|g|}-u^{2|g|}],$$

and $\Gamma(a,b)$ is the incomplete Γ function. For Q near zero, the susceptibility has a power-law Q dependence, but is finite and has a cusp maximum at $Q=0$. Similar results for the ω and T dependence can be readily derived.

IV. PAIRING FLUCTUATIONS

The conventional theory of pairing fluctuations involves the two-particle propagator or pair susceptibility. Successful theories of one-dimensional fluctuations for thin whiskers have been given, using a Ginzburg-Landau functional to describe these order-parameter fluctuations. An extension of these ideas to one-dimensional systems has also been proposed.[5] However, there is a fundamental distinction between a three-dimensional system, with one-dimensional order-parameter fluctuations, and a genuine one-dimensional system. The former is three dimensional from the point of view of interparticle interactions and can support conventional one-dimensional fluctuations because of the large coherence length. We shall see that the latter can be quite different.

The difference is illustrated by the pair propagator $P(q,\omega)$, defined by

$$P(q,\omega)=\int_0^\infty(dt/i)e^{i\omega t}\langle[P_q(t),P_{-q}]\rangle, \tag{32}$$

where

$$P_q=\int dx e^{iqx}L^{-1}\sum_k a^\dagger_{1,k+q}a^\dagger_{2,-k}$$

is the pair operator, spin labels have been suppressed, and time evolution as well as thermal averaging is with the full H of Eq. (2). $P(q,t)$ is the Fourier transform of $P(x,t)$, defined by

$$P(x,t)=-i\Theta(t)\langle[\psi_1(x,t)\psi_2(x,t),\psi_2^\dagger\psi_1^\dagger]\rangle.$$

Using the operators $O_1(x,t)$ and $O_2(x,t)$ as in Eq. (23), the computation of $P(x,t)$ is reduced to familiar algebra.[10] The result is

$$P(x,t)=-i\Theta(t)(2\pi\alpha)^{-2}\{\exp[U(x,t)+U(x,-t)]-(x\to-x,t\to-t)\}, \tag{33}$$

provided $\sinh\varphi$ in the definition of $U(x,t)$ following Eq. (23) is replaced by $-\sinh\varphi$. Except for the phase factor, these two equations are equal, thus $P(q,\omega)=\chi(q-2k_F,\omega)$ with a change in the sign of the interaction potential. The results of Sec. IV can therefore be used to determine $P(q,\omega)$.

An attractive interaction produces a divergent $P(0,0)$ as $T\to0$, indicative of strong pairing fluctuations at low temperatures. Indeed these can be expected to produce enhancement of transport coefficients. It is interesting to note that either P or χ is divergent for the interacting system, as $T\to0$, indicative of a strong tendency towards either a particle-particle or particle-hole instability.

V. DISCUSSION

Before exploring the consequences of our results, it is necessary to recall the relation of the Luttinger and Tomonaga models to real one-dimensional systems. The solution discussed here would only be of academic interest if these models proved to be deficient in some important respect. It is generally believed that these models are good descriptions of reality provided the interaction is sufficiently long ranged. That can be understood from the form of the interaction Hamiltonian, Eq. (2). Consider a pair state in the real system, consisting of particles of momenta near $+k_F$ and $-k_F$. This pair state can scatter to another pair state with momenta near the original, which is a small momentum process. A large momentum scattering may occur, with $k_F \to -k_F$ and $-k_F \to k_F$. With Eq. (2), the corresponding pair state is constructed by a particle in branch 1 near $+k_F$, and a particle in branch 2 near $-k_F$. This pair state scatters according to $1 \to 1$ and $2 \to 2$, which is the small-momentum process, but the $1 \to 2$ and $2 \to 1$ large-momentum process does not occur.

In order for the large-momentum processes to be negligible, it is necessary for the interaction strength to be very small at $\sim 2k_F$, which is the typical momentum transfer involved for the $1 \to 2$, $2 \to 1$ pair transition at the Fermi energy. However, our results have important application even if this is not the case. Any treatment which omits the small-momentum processes will be plagued with $\ln\omega$ singularities, as discussed in Sec. II. A perturbation expansion about our solution might be expected to be a reasonable approximation for these systems with appreciable interaction strength at large momenta.

It is important to recognize the limitations of the quasiparticle approximations used in a recent fluctuation theory of the Peierls instability. Examination of Eq. (29) indicates that departures from free-particle behavior in the small-Q and small-ω region occur when $(Tc^{-1}\alpha)^{2\epsilon}$ differs appreciably from unity. Because $c\alpha^{-1}$ is of the order of a bandwidth, $T\alpha c^{-1}$ is typically 10^{-3} or smaller, leading to significant deviations from unity for quite modest interactions, $g \sim 0.2$. Requiring $(T\alpha c^{-1})^{2\epsilon} \sim e^{-1}$, determines a characteristic $T_0 \sim c\alpha^{-1}e^{-1/2\epsilon}$.

Also, the effects of weak interactions between one-dimensional strands or finite length might be expected to be important in real systems. Although we have not analyzed these in detail, it is plausible that they could introduce an "effective temperature", T^*, into the problem, that is, a low-energy cutoff which removes the low-temperature singularities. For the finite chain, $T^* \sim 2\pi L^{-1}c$, while T^* for interchain coupling is presumably of the order of the coupling strength itself. It is still quite easy for $(T^*c^{-1}\alpha)^{2\epsilon}$ to depart significantly from unity, indicating the interactions studied in this paper to be important. These questions, however, deserve a more careful analysis than presented here.

It is interesting to consider the complete Hamiltonian for the interacting system coupled to the phonons.[12] Using the field operators $O_1(x)$ and $O_2(x)$ defined by Eq. (5) and in the text preceeding Eq. (22), we find

$$H_L = H + \sum_{q,\lambda} \omega_{q\lambda} b^\dagger_{q\lambda} b_{q\lambda} + \sum_{q,\lambda} \int dx e^{iq\cdot x} g_L(q,\lambda) \times [O_1^\dagger(x) O_2(x)(b_{q\lambda} + b^\dagger_{-q\lambda}) + \text{H. c.}] , \qquad (34)$$

where H is the Hamiltonian of Eq. (2), $\omega_{q\lambda}$ and $b_{q\lambda}$ refer to the lattice phonons, the $g_L(q,\lambda)$ is the coupling constant. Following the discussion of Sec. II, and Ref. (6), H can be represented entirely in terms of the boson density operators $\rho_1(p)$ and $\rho_2(p)$. Equation (34) is thus a Hamiltonian defined entirely in the space of these bosons. This new model for the Peierls instability incorporates all the physics of the original system, but has eliminated all reference to the fermion operators. It can be shown, to lowest order in $g_L(g,\lambda)$, that the phonon mass operator is proportional to $\chi(q,\omega)$, indicated by Eq. (21). Equation (34) appears to be particularly suitable for studying corrections to this lowest-order approximation and exploring the real nature of the Peierls instability.

Note added in manuscript. After submitting this paper for publication, we were informed that D. C. Mattis has independently introduced an operator equivalent to $O_1(x)$ [Eq. (5)] in the limit $\alpha \to 0$. He used this operator to study backward scattering from impurities in the Luttinger model.[13]

Note added in proof. An earlier calculation of $G(x,t)$ has been given by Carl Dover.[14] In comparison, our method has the virtue of simplicity and easy extension to finite temperature. The first published prediction that χ and P exhibit power laws, is due to Solyom,[15] using arguments based on perturbation theory, in agreement with our exact solution in the weak coupling limit.

ACKNOWLEDGMENTS

We wish to acknowledge many stimulating discussions with P. Fulde and W. Dieterich. One of us (A. L.) wishes to acknowledge the hospitality of the Institut Max von Laue-Paul Langevin where this work originated.

*Supported in part by the National Science Foundation.

[1] L. B. Coleman, M. J. Cohen, D. J. Sandman, F. G. Yamagishi, A. F. Garito, and A. J. Heeger, Solid State Commun. 12, 1125 (1973).

[2] H. R. Zeller, Adv. Solid State Phys. 13, 31 (1973).

[3] M. J. Rice and S. Strässler, Solid State Commun. 13, 125 (1973).

[4] P. A. Lee, T. M. Rice, and P. W. Anderson, Phys. Rev. Lett. 31, 462 (1973).

[5] P. W. Anderson, P. A. Lee, and M. Saitoh, Solid State Commun. 13, 697 (1973).

[6] Daniel C. Mattis and Elliot H. Lieb, J. Math. Phys. 6, 304 (1965). These methods have been extended to the Tomonaga model by H. Gutfreund and M. Schick [Phys. Rev. 168, 418 (1968)]..

[7] P. Nozières and C. T. de Dominicis, Phys. Rev. 178, 1097 (1969).

[8] K. D. Schotte and U. Schotte, Phys. Rev. 182, 479 (1969).

[9] To be precise the operator identities involving $O_1(x)$ are

only exact in the limit $\alpha \to 0$, which is in fact taken in subsequent calculations.

[10]K. D. Schotte, Z. Phys. 230, 99 (1970). M. Blume, V. J. Emery, and A. Luther, Phys. Rev. Lett. 25, 450 (1970).

[11]We make use of the well-known operator identities $e^A e^B = \exp(A + B + [A, B]/2)$ and $\langle e^A \rangle = e^{\langle A^2 \rangle /2}$, where A and B are linear combinations of boson creation and destruction operators and the average is in a harmonic oscillator density matrix.

[12]The effects of phonons on BCS pairing in a one-dimensional system have been considered by B. R. Patton and L. J. Sham [Phys. Rev. Lett. 31, 631 (1973)].

[13]Daniel C. Mattis, report of work prior to publication.

[14]Carl B. Dover, Ann. Phys. (N. Y.) 50, 500 (1968).

[15]J. Solyom, J. Low Temp. Phys. 12, 529 (1973).