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BACKSCATTERING IN THE ONE-DIMENSIONAL MANY-FERMION SYSTEM

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The Sawada Hamiltonian model is generalized to include the backscattering interaction in a one-dimensional many-fermion system. The collective excitations of the particle-density fluctuations and the backscattering dielectric function are obtained. It is shown that the giant Kohn anomaly of the longitudinal phonon spectrum, observed in the quasi-one-dimensional conductors, is qualitatively reproduced within the present approach.

1. INTRODUCTION

THE LOW EXCITED states of the non-interacting one-dimensional many-fermion system can be constructed with particle–hole pairs which involve single-particle states in the neighbourhood of the two $\pm k_F$ Fermi points (k_F being the Fermi momentum). In order to get a precise description of these states we shall restrict ourselves to those single-particle states whose wave-vector p runs within the range $-k_F-k_c<p<-k_F+k_c$ and $+k_F-k_c<p<+k_F+k_c$, where k_c is the bandwidth cut-off, much smaller than k_F. A linear p-dependence can readily be obtained for the unperturbed energy levels of these single-particle states: $\epsilon_p=\epsilon_F+v_F(|p|-k_F)$, where ϵ_F is the Fermi level and v_F is the Fermi velocity. Much theoretical work, recently reviewed by Sólyom [1], relied on this simple relationship which is the essential feature of the model.

In the one-dimensional many-fermion system as formulated above there are two types of interaction processes. The first one is the forward scattering process that involves a small momentum transfer. This process excites one particle–hole pair in the neighbourhood of $+k_F$ and another one in the neighbourhood of $-k_F$. The second one is the backscattering process, with momentum transfer near $2k_F$, that excites two particle–hole pairs across the Fermi sea. One can see that the excitation energies involved in both processes are very small. Consequently, the dynamics of the system is governed both by the forward scattering and backscattering process.

The forward scattering interaction has been treated within the Tomonaga–Luttinger model [2–5]. The backscattering interaction has been studied by means of both the bosonization technique [6] and renormalization group approach [7]. A remarkable exact solution has been given by Luther and Emery [6] in the case of attractive interaction for a particular value of the backscattering coupling constant. Within the renormalization group approach the vertex part (scattering amplitude) has been calculated for a particular choice of its external variables ($\pm k_F$) [1]. This quantity is very useful for treating the various instabilities of the system but it is more difficult to be used for getting the dispersion relation of the particle-density excitations.

The aim of this paper is to study the backscattering process with repulsive spin–independent interaction [8]. Our approach is based upon the Sawada Hamiltonian model which has been employed [9] for treating the long-range interaction in the three-dimensional electron gas. This approach is slightly modified in order to study the forward scattering in the one-dimensional system and is generalized to include the backscattering interaction. The dispersion relations of the particle-density excitations as well as the backscattering dielectric function are obtained. It is shown that the giant Kohn anomaly, observed in the longitudinal phonon spectrum of the quasi-one-dimensional conductors, is reproduced by our approach. A possible connection is discussed between our results and the optical data of the quasi-one-dimensional conductors.

2. FORWARD SCATTERING

The system of interacting fermions is described by the Hamiltonian

$$H = H_0 + H_1,$$

$$H_0 = \sum_p \epsilon_p c_p^+ c_p,$$

$$H_1 = \frac{1}{2}\sum_{kp_1p_2} v(k) c^+_{p_1+k} c^+_{p_2-k} c_{p_2} c_{p_1}, \qquad (1)$$

where $c_p^+(c_p)$ is the creation (annihilation) operator of

the p-fermion state and $v(k)$ is the Fourier transform of the interaction. Although the spin index is omitted in equation (1) the spin contribution (a factor 2) will be considered in counting the single-particle states.

It is well known [9] that the basic quantities in the Sawada Hamiltonian model are the creation and annihilation operators of the particle–hole pairs. These operators are of the form $c^+_{p+k}c_p$ where p lies inside and $p+k$ outside the Fermi sea. As we shall restrict ourselves to the low excited state the wave-vectors p and $p+k$ will be confined to small regions around the Fermi points, defined by the bandwidth cut-off k_c. Using the linear p-dependence of the unperturbed single-particle energy levels it is easy to see that the excitation energy of a particle-hole pair with small momentum transfer (forward scattering) depends on the momentum transfer only. Consequently, it is convenient to use a superposition of particle–hole pairs operators defined by

$$A^+_{1k} = g_k^{-1} \sum_{p\in\delta_1} c^+_{p+k}c_p, \quad A^+_{2k} = g_k^{-1} \sum_{p\in\delta_2} c^+_{p-k}c_p, \tag{2}$$

and the corresponding annihilation operators. In equation (2) the regions δ_1 and δ_2 are given by

$$\delta_1 = \begin{cases} k_F - k < p < k_F, & 0 < k < k_c, \\ k_F - k_c < p < k_F + k_c - k, & k_c < k < 2k_c, \end{cases}$$
$$\delta_2 = \begin{cases} -k_F < p < -k_F + k, & 0 < k < k_c, \\ -k_F - k_c + k < p < -k_F + k_c, & k_c < k < 2k_c, \end{cases} \tag{3}$$

and the normalization factor

$$g_k = \begin{cases} (k/\pi)^{1/2}, & 0 < k < k_c, \\ [(2k_c - k)/\pi]^{1/2}, & k_c < k < 2k_c \end{cases} \tag{4}$$

is chosen so as $\langle 0|A_{1k}A^+_{1k}|0\rangle = \langle 0|A_{2k}A^+_{2k}|0\rangle = 1$, $|0\rangle$ being the ground state of the non-interacting system. For commutation relations of the A-operators the averages will be used of their commutators on the non-interacting ground state $|0\rangle$. This approximation, which is the characteristic feature of the Sawada Hamiltonian model, is valid in the limit of weak coupling strengths when the interaction does not distort appreciably the Fermi sea of the system [4, 5, 10]. Using this approximation we get boson-like commutation relations $[A_{1k}, A^+_{1k'}] = [A_{2k}, A^+_{2k'}] = \delta_{kk'}$ and $[A_{1k}, A_{2k'}] = 0$.

With the linearized form for ϵ_p we obtain the commutators of the kinetic Hamiltonian H_0 [equation (1)] with the operators A^+_{1k} and A^+_{2k}:

$$[H_0, A^+_{1k}] = v_F k A^+_{1k}, \quad [H_0, A^+_{2k}] = v_F k A^+_{2k}, \tag{5}$$

so that the following expression can be used instead of H_0:

$$H_{0f} = \sum_{0<k<2k_c} v_F k (A^+_{1k}A_{1k} + A^+_{2k}A_{2k}). \tag{6}$$

Looking for the forward scattering processes the interaction Hamiltonian H_1 [equation (1)] can be written as (up to a constant term)

$$H_{1f} = v \sum_{0<k<2k_c} g_k^2 (A^+_{1k}A_{1k} + A^+_{2k}A_{2k} + A^+_{1k}A^+_{2k} + A_{1k}A_{2k}), \tag{7}$$

where the interaction has been taken as constant $v(k) = v$, for small k, $0 < k < 2k_c$. The full Hamiltonian $H_f = H_{0f} + H_{1f}$ of the forward scattering can straightforwardly by diagonalized by means of the Mattis and Lieb unitary transformation [4]. We get the dispersion relation of the particle-density excitations associated with the forward scattering process:

$$\omega(k) = \begin{cases} v_F k(1 + 2v/\pi v_F)^{1/2}, & 0 < k < k_c, \\ \left[v_F^2 k^2 + \dfrac{2}{\pi} v v_F k(2k_c - k)\right]^{1/2}, & k_c < k < 2k_c. \end{cases} \tag{8}$$

For $0 < k < k_c$ this dispersion relation has previously been derived [2, 4, 5] by various techniques.

3. BACKSCATTERING

We introduce the excitation operators of the backscattering particle–hole pairs

$$b^+_{1p}(k) = c^+_{p+2k_F+k}c_p, \quad p\in\delta_3,$$
$$b^+_{2p}(k) = c^+_{p-2k_F-k}c_p, \quad p\in\delta_4, \tag{9}$$

(and the corresponding annihilation operators) where the regions

$$\delta_3 = \begin{cases} -k_F < p < -k_F + k_c - k, & 0 < k < k_c, \\ -k_F - k < p < -k_F + k_c, & -k_c < k < 0, \end{cases}$$
$$\delta_4 = \begin{cases} k_F - k_c + k < p < k_F, & 0 < k < k_c, \\ k_F - k_c < p < k_F + k, & -k_c < k < 0 \end{cases} \tag{10}$$

have been chosen so as to have $-k_F < p < -k_F + k_c$, $k_F < p + 2k_F + k < k_F + k_c$ for the first set of operators $[b^+_{1p}(k), b_{1p}(k)]$ and $k_F - k_c < p < k_F$, $-k_F - k_c < p - 2k_F - k < -k_F$ for the second one $[b^+_{2p}(k), b_{2p}(k)]$. The approximate commutation relations of these operators are obtained, as in the case of the forward scattering, by taking the averages of their commutators on the non-interacting ground state $|0\rangle$. We get boson-like commutation relations

$$[b_{1p}(k), b^+_{1p'}(k')] = [b_{2p}(k), b^+_{2p'}(k')] = \delta_{pp'}\delta_{kk'},$$
$$[b_{1p}(k), b_{2p'}(k')] = 0 \tag{11}$$

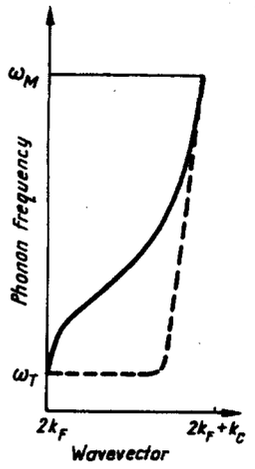

Fig. 1. The $2k_F$ anomaly for KCP reported by Carneiro *et al.* [11] (dashed curve) and given by equation (20) (full curve). The parameters in equation (20) have been taken from the experimental data [11] at $T = 160$ K ($\omega_M = 8$ meV, $\omega_T = 3.1$ meV, $k_c = 6.68 \times 10^{-3}$ Å^{-1}, the slope at $k_c = 0.7 \times 10^5$ m sec^{-1}, $v_F = 11 \times 10^5$ m sec^{-1}). With these data we get for the electron–electron interaction $u/2\pi v_F = 2.82$ and for the parameter $\alpha = \exp(-2\pi v_F/u)$ the value 0.7.

and all the b-operators commute with the A-operators.

The commutators of the kinetic Hamiltonian H_0 with the operators $b^+_{1p}(k)$ and $b^+_{2p}(k)$ are

$$\begin{aligned}[H_0, b^+_{1p}(k)] &= \omega_p(k) b^+_{1p}(k),\\ [H_0, b^+_{2p}(k)] &= \omega_{-p}(k) b^+_{2p}(k),\end{aligned} \tag{12}$$

where $\omega_p(k) = v_F(2k_F + 2p + k)$ was obtained by using the linearized form of the unperturbed single-particle energy levels. It results that the backscattering kinetic Hamiltonian can be written as

$$H_{0,b} = \sum_{pk} [\omega_p(k) b^+_{1p}(k) b_{1p}(k) + \omega_{-p}(k) b^+_{2p}(k) b_{2p}(k)]. \tag{13}$$

In the interaction Hamiltonian H_1 we shall pick out those terms which describe the backscattering process, that is the terms with momentum transfer near $\pm 2k_F$. Then the interaction Hamiltonian becomes (up to a constant term)

$$\begin{aligned}H_{1b} = u \sum_{kp_1p_2} &[b^+_{1p_1}(k) + b_{2p_1}(k)]\\ &\times [b^+_{2p_2}(k) + b_{1p_2}(k)],\end{aligned} \tag{14}$$

where the interaction has been taken as constant, $v(2k_F + k) = v(-2k_F - k) = u$, for small k, $-k_c < k < k_c$. We emphasize here that the p-subscripts of the b_1- and b_2-operators in the H_{0b} and H_{1b} should be taken inside the regions δ_3 and δ_4, respectively. The full Hamiltonian $H_b = H_{0b} + H_{1b}$ of the backscattering process can easily be brought into the diagonalized form

$$H_b = \sum_k \omega(k)(B^+_{1k}B_{1k} + B^+_{2k}B_{2k}) \tag{15}$$

by means of the well-known [9] unitary transformation

$$\begin{aligned}B^+_{1k} = \text{const} \Bigg\{ &\sum_{p\in\delta_3} [\omega - \omega_p(k)]^{-1} b^+_{1p}(k)\\ &+ \sum_{p\in\delta_4} [\omega + \omega_{-p}(k)]^{-1} b_{2p}(k) \Bigg\},\end{aligned} \tag{16}$$

$$\begin{aligned}B^+_{2k} = \text{const} \Bigg\{ &\sum_{p\in\delta_4} [\omega - \omega_{-p}(k)]^{-1} b^+_{2p}(k)\\ &+ \sum_{p\in\delta_3} [\omega + \omega_p(k)]^{-1} b_{1p}(k) \Bigg\},\end{aligned}$$

if ω obeys the condition

$$\begin{aligned}\epsilon(k,\omega) = 1 - u \Bigg\{ &\sum_{p\in\delta_3} [\omega - \omega_p(k)]^{-1}\\ &- \sum_{p\in\delta_4} [\omega + \omega_{-p}(k)]^{-1} \Bigg\} = 0,\end{aligned} \tag{17}$$

$\epsilon(k, \omega)$ being the backscattering dielectric function. By performing the summations in equation (17) we get

$$\epsilon(k,\omega) = 1 + \frac{u}{2\pi v_F} \ln \left| \frac{\omega^2 - v_F^2(2k_c - |k|)^2}{\omega^2 - v_F^2 k^2} \right|, \quad |k| < k_c, \tag{18}$$

whence

$$\omega(k) = v_F[k^2 + 4k_c(k_c - |k|)/(1 \mp \alpha)]^{1/2}, \quad |k| < k_c, \tag{19}$$

with $\alpha = \exp(-2\pi v_F/u)$. This is the dispersion relation of the particle-density excitations induced by the backscattering interaction. For repulsive interaction $\alpha < 1$ the frequency given by equation (19) exhibits a gap at $k = 0$ (momentum transfer $2k_F$) of magnitude $2v_F k_c (1 \mp \alpha)^{-1/2}$. For attractive interaction $\alpha > 1$ the branch of the frequency which contains $1 - \alpha$ becomes imaginary at wavevectors smaller than $2k_c(\sqrt{\alpha} + 1)^{-1}$. This result points out an instability of the system against attractive backscattering interaction.

4. KOHN ANOMALY

The neutron scattering experiments performed on KCP [11] and TTF–TCNQ [12] revealed the softening of the $2k_F$ phonons in these quasi-one-dimensional conductors above and below the metal–insulator transition temperature. This anomaly is caused by the electron–electron backscattering process (via electron–phonon coupling) and it has been shown [13] that the dip around $2k_F$ in the dispersion relation of the longitudinal acoustic phonons should be considerably

pronounced in the one-dimensional system (giant Kohn anomaly). The experimental curve obtained by Carneiro *et al.* [11] for KCP is shown in Fig. 1 (dashed line), where ω_M is the unperturbed phonon frequency and ω_T is the minimum frequency of the distorted phonons. The screened frequency of the longitudinal acoustic phonons with wavevector near $2k_F$ may be written as [14]

$$\omega_{ph}(k) = \omega_T\{1 + [(\omega_M/\omega_T)^2 - 1]\epsilon^{-1}(k, 0)\}^{1/2}, \quad (20)$$

where $\epsilon(k, 0)$ is the backscattering dielectric function of zero frequency given by equation (18). This formula reproduces qualitatively (full line in Fig. 1) the experimental curve if the electron–electron interaction u in equation (18) is taken so as the both curves have the same slope at k_c. The finite phonon life-time is responsible for the flat bottom of the dashed curve and we expect that a consistent theory of the electron–phonon interaction (including the backscattering electronic process) in these materials will be able to account for this feature of the experimental curve and for its slight temperature dependence as well.

Using the experimental data for KCP [11] at $T = 60$ K and $T = 160$ K we get for the two gap values of the backscattering electron-density excitations [equation (19) for $k = 0$] the values 0.23 and 0.12 eV and, respectively, 1.12 and 0.47 eV. We suggest that these backscattering excitations of the electrons might be responsible for the optical gap of 0.2 eV and for the low-lying optical mode of 1.9 meV observed in this material [15]. We also mention here that the experimental large low-temperature dielectric constant in TTF–TCNQ [16] is consistent with our equation (18) at low frequencies.

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