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Electron–phonon coupling in one dimension

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Abstract. The Ward identity is derived for the electron–phonon coupling in one dimension and the spectrum of elementary excitations is calculated by assuming that the Fermi distribution is not strongly distorted by the interaction. The electron–phonon vertex is renormalised in the case of the forward scattering and Migdal's theorem is discussed. A model is proposed for the giant Kohn anomaly. The dip in the phonon spectrum is obtained and compared with the experimental data for KCP.

1. Introduction

Recently there has been considerable interest in the electron–phonon coupling in the one-dimensional many-electron systems, especially in connection with the instabilities of the nearly one-dimensional conductors toward both dynamic and structural changes (for a recent review see, for example, Devreese *et al* 1979).

The chain-like structure of the lattice of these materials confines the motion of the electrons to one direction in space and this permits the linearisation of the momentum dependence of the free-electron levels within two finite regions centred around $\pm k_F$, k_F being the Fermi momentum. The linear spectrum of the single-electron states near $\pm k_F$ produces high divergencies in the relevant quantities (logarithmic singularities) and this results in an unusual behaviour of the one-dimensional conductors. Most of the phenomena generally occurring for all condensed matter systems are strongly enhanced in this materials. Therefore, it is important to see to what extent the above-mentioned singularities will be reflected in the physical behaviour of the systems. Particularly interesting is the giant Kohn anomaly observed in the phonon spectrum near $2k_F$ and the associated softening of the phonon modes. This strong distortion of the phonon spectrum in one dimension has been investigated by Afanas'ev and Kagan (1963). It was shown that this effect originates in a sharp increase in the number of low-energy states available for the electron–hole excitation accompanied by the absorption or emission of phonons with wavevectors near $2k_F$.

The aim of the present paper is to investigate the electron–phonon interaction in the one-dimensional many-electron system within the perturbation theoretical approach. An electron gas model is proposed having explicitly introduced a band-width cut-off. As the low excited states of the system consist of electron–hole pairs in the neighbourhood of the $\pm k_F$ points we restrict ourselves to these single-electron states only. Their

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wavevectors p run within the range $\pm k_F - k_c < p < \pm k_F + k_c$, where k_c is the band-width cut-off, much smaller than k_F. The energy levels ε_p of the electron states can be linearised as follows: $\varepsilon_p = \mu + v_F(|p| - k_F)$, where μ is the Fermi level and v_F is the Fermi velocity. Two types of electron–phonon interaction processes may take place in this model. The first is the forward scattering process, that excites an electron–hole pair near $\pm k_F$ by creating or absorbing a virtual phonon of small wavevector. The second is the backscattering process in which the electron–hole pair excited across the Fermi sea is accompanied by the emission or absorption of a phonon with wavevector near $2k_F$.

Our approach relies upon the Ward identity which connects the electron–phonon vertex to the electron Green function. This identity is a direct consequence of the linear electron spectrum and of the conservation of the number of electrons near $\pm k_F$. The Ward identity is derived here by means of the equation-of-motion method in a manner analogous to that used for the electron–electron interaction (Apostol 1981a). For the forward scattering process this is an exact result, extensively used in studying the electron–electron interaction in one-dimensional systems (Dzialoshinsky and Larkin 1973, Everts and Schulz 1974). The Ward identity is generalised here to the back-scattering process in the limit of weak coupling, that is when the ground state is not too strongly distorted by interaction. The Ward identity is particularly suitable for treating our model as it allows us to control at every step the confinement of the electron wavevectors to the two regions around $\pm k_F$. Moreover, it can be used to get a simple, physical meaning of the approximations made in working out the complete set of integral equations of the perturbation theory.

The polarisation and the normal modes are calculated both for the forward and backward scattering processes assuming that the interaction does not distort appreciably the Fermi sea. The Ward identity is used to renormalise the electron–phonon vertex and to check the validity of Migdal's theorem in the case of the forward scattering. It is shown that, unlike the three-dimensional case, the electron dressing is $O(m/M)$, m and M being the electronic and ionic mass, respectively. The electrons may be considered to a good approximation as undressed in comparison with the phonons. Particular attention is paid to the phonon modes of wavevectors near $2k_F$. The giant dip of the Kohn anomaly is obtained within our model and compared with the experimental data for KCP. It is shown that the band-width cut-off k_c plays an essential role in describing this strong distortion of the phonon spectrum. We should remark that similar calculations have been attempted by Horovitz *et al* (1974). As they were interested only in the drastic effects, they used an unrealistic model in which the cut-off parameter does not appear. This is why their results cannot be compared with the experiments. Our calculations, made for the case of KCP, are in agreement with the experimental data.

The paper is organised as follows. The Ward identity is derived in § 2. The forward scattering process and the Migdal theorem are discussed in § 3. In § 4 the backscattering process is analysed and the dip is obtained in the phonon spectrum of KCP. The conclusions are given in § 5.

2. Ward identity for the electron–phonon coupling in one dimension

Let us assume a one-dimensional electron–phonon system described by the Fröhlich type Hamiltonian

$$H = \sum_p \varepsilon_p c_p^+ c_p + \sum_q \omega_q b_q^+ b_q + g \sum_{p,q} (\omega_q/2)^{1/2} (b_q + b_{-q}^+) c_{p+q}^+ c_p, \tag{1}$$

where $c_p(c_p^+)$ and $b_q(b_q^+)$ are electron and phonon destruction (creation) operators, respectively, ε_p is the free electron energy, $\omega_q = c|q|$ is the bare phonon frequency (c being the unrenormalised sound velocity) and g is the bare electron–phonon coupling constant. The spin index will be omitted throughout, but the spin contribution (a factor 2) will be considered in counting the single-electron states.

We define the three-point vertex function

$$K(x_1, x_2, x_3) = \langle T\{[n(x_1) - \langle n(x_1)\rangle]\ \psi^+(x_2)\ \psi(x_3)\}\rangle, \tag{2}$$

where $\langle \ldots \rangle$ means average over the Heisenberg ground state, T is the time ordering operator, x denotes the space–time coordinate pair (x, t), $\psi(x)$ is the electron field operator written in the plane wave representation, $\psi(x) = \Sigma_p c_p \exp(ipx)$ and $n(x) = \psi^+(x)\ \psi(x)$ is the electron density operator. All the operators in (2) are written in the Heisenberg picture. Due to the space–time invariance of the system this function depends only on two arguments. Choosing $x_2 - x_1$ and $x_3 - x_2$ as independent variables, the three-point vertex function can be Fourier transformed as

$$K(x_2 - x_1, x_3 - x_2) = (2\pi)^{-4} \int \mathrm{d}p\ \mathrm{d}q\ K(p, q) \exp[ip \cdot (x_3 - x_2)] \exp[iq \cdot (x_2 - x_1)],$$

$$\begin{aligned} K(p, q) = \sum_{p_1} \int \mathrm{d}(t_2 - t_1)\ \mathrm{d}(t_3 - t_2)\ \langle T\{[c_{p_1}^+(t_1)\ c_{p_1 - q}(t_1) \\ - \langle c_{p_1}^+(t_1)\ c_{p_1 - q}(t_1)\rangle]\ c_{p-q}^+(t_2)\ c_p(t_3)\}\rangle \\ \times \exp[i\omega(t_2 - t_1)] \exp[i\varepsilon(t_3 - t_2)], \end{aligned} \tag{3}$$

where $p = (p, \varepsilon)$, $q = (q, \omega)$ and the scalar product is taken as usually $p \cdot x = px - \varepsilon t$, $q \cdot x = qx - \omega t$, The Fourier transform $K(p, q)$ can be expressed by the connected diagrams drawn in figure 1. The reducible diagrams in this figure (that can be split into two distinct parts by cutting a single phonon line) are given by

$$K_{\mathrm{red}}(p, q) = g^{-1} G(p)\ G(p - q)\ \Gamma(p, q)\ D(q)\ \Pi(q), \tag{4}$$

whereas the irreducible diagrams have the analytic expression

$$K_{\mathrm{irred}}(p, q) = g^{-1} G(p)\ G(p - q)\ \Gamma(p, q). \tag{5}$$

In (4) and (5) $G(p)$ and $D(q)$ are the electron and phonon Green functions, respectively, $\Pi(q)$ is the irreducible polarisation and $\Gamma(p, q)$ is the three-legged vertex function. This

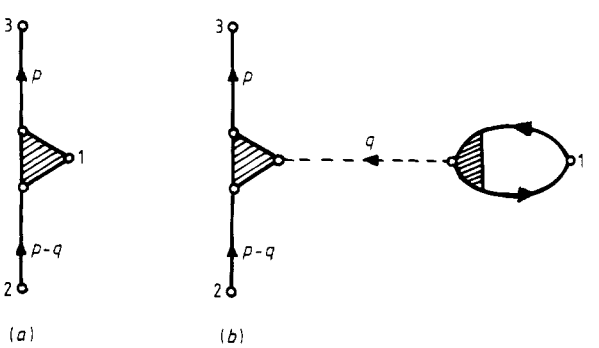

Figure 1. Irreducible (a) and reducible (b) diagrams of the three-point vertex function $K(p, q)$. The hatched triangle represents the three-legged vertex function $\Gamma(p, q)$.

vertex function represents all the connected irreducible diagrams with three external legs. Taking the derivative of (2) and (3) with respect to the first time argument, using the Heisenberg equation of motion for the operator $n(x_1)$, and comparing the results we get

$$\sum_{p_1}(\omega-\varepsilon_{p_1}+\varepsilon_{p_1-q})\int \mathrm{d}(t_2-t_1)\,\mathrm{d}(t_3-t_2)\,\langle T\{[c^+_{p_1}(t_1)\,c_{p_1-q}(t_1)$$
$$-\langle c^+_{p_1}(t_1)\,c_{p_1-q}(t_1)\rangle]\,c^+_{p-q}(t_2)\,c_p(t_3)\}\rangle$$
$$\times\exp[\mathrm{i}\omega(t_2-t_1)]\exp[\mathrm{i}\varepsilon(t_3-t_2)]$$
$$=G(\boldsymbol{p}-\boldsymbol{q})-G(\boldsymbol{p}). \tag{6}$$

One can easily find that the analytic expression of the reducible diagrams associated with the averaged operator product in (6) is given by

$$\langle T\{[c^+_{p_1}(t_1)\,c_{p_1-q}(t_1)-\langle c^+_{p_1}(t_1)\,c_{p_1-q}(t_1)\rangle]\,c^+_{p-q}(t_2)\,c_p(t_3)\}\rangle_{\mathrm{red}}$$
$$=-\mathrm{i}g^2\int \mathrm{d}t'\,\mathrm{d}t''\,D_0(q,t'-t'')\,\langle T\{[c^+_{p_1}(t_1)\,c_{p_1-q}(t_1)$$
$$-\langle c^+_{p_1}(t_1)\,c_{p_1-q}(t_1)\rangle]\rho_q(t'')\}\rangle$$
$$\times\langle T\{[\rho_{-q}(t')-\langle\rho_{-q}(t')\rangle]\,c^+_{p-q}(t_2)\,c_p(t_3)\}\rangle_{\mathrm{irred}}, \tag{7}$$

where $D_0(\boldsymbol{q})=\omega_q^2(\omega^2-\omega_q^2+\mathrm{i}\delta)^{-1}$ is the free phonon Green function and ρ_q is the Fourier transform of the electron density operator. Let us introduce the electron-density correlation function

$$N(\boldsymbol{x}'-\boldsymbol{x})=-\mathrm{i}\langle T\{[n(\boldsymbol{x})-\langle n(\boldsymbol{x})\rangle]\,n(\boldsymbol{x}')\}\rangle$$
$$=(2\pi)^{-2}\int \mathrm{d}q\,N(q)\exp[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{x}'-\boldsymbol{x})]. \tag{8}$$

In the same way as for the three-point vertex function we obtain the following equation of motion for this function:

$$\sum_{p_1}(\omega-\varepsilon_{p_1}+\varepsilon_{p_1-p})\int \mathrm{d}(t'-t)\,\langle T\{[c^+_{p_1}(t)\,c_{p_1-q}(t)-\langle c^+_{p_1}(t)\,c_{p_1-q}(t)\rangle]$$
$$\times\rho_q(t')\}\rangle\exp[\mathrm{i}\omega(t'-t)]=0. \tag{9}$$

Using this result and (7) one can easily see that the reducible diagrams do not contribute to (6), which can now be written as

$$\sum_{p_1}(\omega-\varepsilon_{p_1}+\varepsilon_{p_1-q})\int \mathrm{d}(t_2-t_1)\,\mathrm{d}(t_3-t_2)\,\langle T\{[c^+_{p_1}(t_1)\,c_{p_1-q}(t_1)$$
$$-\langle c^+_{p_1}(t_1)\,c_{p_1-q}(t_1)\rangle]\,c^+_{p-q}(t_2)\,c_p(t_3)\}\rangle_{\mathrm{irred}}$$
$$\times\exp[\mathrm{i}\omega(t_2-t_1)]\exp[\mathrm{i}\varepsilon(t_3-t_2)]$$
$$=G(\boldsymbol{p}-\boldsymbol{q})-G(\boldsymbol{p}). \tag{10}$$

The forward scattering processes involve electron–hole pairs in the neighbourhood of the $\pm k_{\mathrm{F}}$ points associated with phonons of small wavevectors $|q|<2k_{\mathrm{c}}$. These processes are described by two vertex functions $\Gamma^{\mathrm{f}}_{\pm}(\boldsymbol{p},\boldsymbol{q})$ corresponding to $p,\,p-q\sim+k_{\mathrm{F}}$ and $p,\,p-q\sim-k_{\mathrm{F}}$, respectively. Restricting ourselves to the single-electron states with wavevectors near $\pm k_{\mathrm{F}}$ it results that p_1 in (10) is also near $\pm k_{\mathrm{F}}$. Under these assumptions

we may use the linear form of the electron energy $\varepsilon_p = \mu + v_F(|p| - k_F)$, so that $\omega - \varepsilon_{p_1} + \varepsilon_{p_1-q}$ becomes $\omega \mp v_F q$. Using (10) and the analytic expression of the irreducible diagrams given by (5) we obtain the Ward identity for the forward scattering

$$g^{-1}\Gamma^f_{\pm}(p, q) = \frac{G^{-1}_{\pm}(p) - G^{-1}_{\pm}(p-q)}{\omega \mp v_F q}, \tag{11}$$

where the upper (lower) sign refers to the forward scattering processes near $+k_F(-k_F)$. It is worth noting that this is an exact result which is still valid in the limit $q \to 0$ in the three-dimensional case (Engelsberg and Schrieffer 1963). A straightforward diagrammatic analysis shows that the Ward identity (11) leads to the exact cancellation of all the diagrams which contain loops with more than two electron lines. The cancellation of these diagrams among themselves (non-Tomonaga diagrams) has been checked by Engelsberg and Varga (1964) to high orders of the perturbation theory. The backscattering processes are described by two vertex functions $\Gamma^b_{\pm}(p, q)$ corresponding to $p \sim +k_F$, $q \sim +2k_F$ and $p \sim -k_F$, $q \sim -2k_F$, respectively. Assuming that the ground state is only slightly modified by interaction we may average in (10) over the non-interacting ground state of the system. Using again the linear form of the electron energy one obtains the backscattering Ward identity

$$g^{-1}\Gamma^b_{\pm}(p, q) = \frac{G^{-1}_{\pm}(p) - G^{-1}_{\mp}(p-q)}{\omega \mp v_F(2p - q)}. \tag{12}$$

We remark that this result could be obtained from (10) by assuming that the backscattering interaction involves only one momentum transfer near $+2k_F$ or $-2k_F$ (which means the random phase approximation). In this case the momentum conservation in the irreducible diagrams shown in figure 1 leads to $p_1 = p$ in (10). It appears that our assumption used for deriving (12) amounts to the random phase approximation. This is a well-known result in the theory of the one-dimensional many-fermion systems (Gutfreund and Schick 1968, Apostol *et al* 1981).

3. Forward scattering and Migdal's theorem

The irreducible polarisation is given by

$$\Pi(q) = -2ig(2\pi)^{-2} \int \mathrm{d}p G(p) G(p-q) \Gamma(p, q). \tag{13}$$

Using the Ward identity for the forward scattering (11) and integrating over energy we get

$$\Pi^f_{\pm}(q) = \frac{g^2}{\pi} \frac{1}{\omega \mp v_F q} \int \mathrm{d}p (n^{\pm}_p - n^{\pm}_{p-q}), \tag{14}$$

where $n^{\pm}_p$ is the momentum distribution of the electrons near $\pm k_F$. As the number of electrons is conserved by interaction the integral in (14) calculated with the step momentum distribution does not differ from that calculated with the real momentum distribution corresponding to the interacting system. Making use of the band-width cut-off k_c one

obtains the irreducible polarisation

$$\Pi^{f}(q) = \Pi^{f}_{+}(q) + \Pi^{f}_{-}(q) = \frac{2}{\pi}\frac{g^2 v_F}{\omega^2 - v_F^2 q^2}A(q), \qquad A(q) = \begin{cases} q^2, & 0 < |q| < k_c, \\ |q|(2k_c - |q|), & k_c < |q| < 2k_c. \end{cases} \tag{15}$$

We remark that the same form of the irreducible polarisation would be obtained from (13) by using the free-electron Green function and the bare electron–phonon vertex $\Gamma_0 = g$. The Ward identity enables us to replace this questionable approximation by a weaker and more reasonable condition, that of the weak coupling. The phonon Green function $D(q)$ and the electron-density correlation function $N(q)$ are given by

$$D^{f}(q) = \frac{D_0(q)}{\Pi^{f}(q)}N^{f}(q) = [D_0^{-1}(q) - \Pi^{f}(q)]^{-1} = \left(\frac{\omega^2 - \omega_q^2}{\omega_q^2} - \frac{2}{\pi}\frac{g^2 v_F}{\omega^2 - v_F^2 q^2}A(q)\right)^{-1}. \tag{16}$$

The poles of this function provide us with the dispersion relaton of the normal modes

$$\Omega_q^2 = \tfrac{1}{2}\{\omega_q^2 + v_F^2 q^2 \pm [(\omega_q^2 - v_F^2 q^2)^2 + 8\lambda v_F^2 \omega_q^2 A(q)]^{1/2}\}, \tag{17}$$

where the dimensionless electron–phonon coupling constant $\lambda = g^2/\pi v_F$ has been introduced and the lifetime effects have been neglected. If we assume, as usual $v_F \gg c$, (17) yields

$$\Omega_q = \omega_q[1 - 2\lambda A(q)/q^2]^{1/2}, \tag{18a}$$

$$\Omega_q = v_F|q|\left(1 + 2\lambda\frac{c^2}{v_F^2}\frac{A(q)}{q^2}\right)^{1/2}. \tag{18b}$$

The excitations given by (18*a*) are dressed phonons. For $|q| < k_c$ the effect of the electron–phonon interaction is a renormalisation of the sound velocity, while for $k_c < |q| < 2k_c$ the momentum dependence is somewhat distorted, the square root in (18*a*) being q-dependent. As regards the excitation described by (18*b*) they are electron–hole pair excitations. Since the sound velocity is proportional to the adiabatic parameter $(m/M)^{1/2}$ one can see from (18*b*) that there is no dressing for the electron–hole pair excitations up to the order of m/M.

We pass now to the study of the Migdal theorem (Migdal 1958) in the one-dimensional system. As is well known, in the three-dimensional case this theorem states that the electron–phonon vertex may be taken of the form $\Gamma = g[1 + O(m/M)^{1/2}]$ if $v_F \gg c$. In the opposite limit, $v_F \ll c$, the vertex corrections are non-negligible and were calculated by Engelsberg and Schrieffer (1963). The first-order correction to the vertex function is given by

$$\Gamma_1(p, q) = ig^2(2\pi)^{-2}\int dp' D_0(p')G_0(p - p')G_0(p - p' - q). \tag{19}$$

The difference between our one-dimensional evaluation and Migdal's three-dimensional one consists in the limitation of the momentum integrations. In the present case all the electronic momenta must be restricted within the ranges $\pm k_F - k_c < p < \pm k_F + k_c$ while in the three-dimensional case the integrations over momenta are restricted by the Debye

momentum cut-off. Performing the integration in (19) we get

$$\Gamma_1(p,q)=\frac{cg^3}{4\pi(\omega-v_Fq)}\left(\frac{p-k_F+k_c}{v_F+c}+\frac{p-2q-k_F+k_c}{v_F-c}\right.$$
$$+\frac{\varepsilon-\mu-\omega-v_F(p-q-k_F)}{(v_F+c)^2}$$
$$\times\ln\left|\frac{\varepsilon-\mu-\omega+c(p-k_F-q)}{\varepsilon-\mu-\omega+c(p-k_F-k_c)-v_Fk_c}\right.$$
$$\left.\times\frac{\varepsilon-\mu-\omega-v_F(p-q-k_F)}{\varepsilon-\mu-\omega+c(p-q-k_F+k_c)+v_Fk_c}\right|$$
$$+\frac{\varepsilon-\mu-\omega-v_F(p-q-k_F)}{(v_F-c)^2}\ln\left|\frac{\varepsilon-\mu-\omega-v_F(p-q-k_F)}{\varepsilon-\mu-\omega-c(p-q-k_F)}\right|$$
$$-\frac{\varepsilon-\mu-v_F(p-k_F)}{(v_F+c)^2}\ln\left|\frac{\varepsilon-\mu+c(p-k_F)}{\varepsilon-\mu+c(p-k_F-k_c)-v_Fk_c}\right|$$
$$\left.-\frac{\varepsilon-\mu-v_F(p-k_F)}{(v_F-c)^2}\ln\left|\frac{\varepsilon-\mu-c(p-q-k_F+k_c)+v_Fk_c}{\varepsilon-\mu-c(p-k_F)}\right|\right) \tag{20}$$

for $0<q<k_c$ and $k_F-k_c<p<k_F+q$ and similar expressions for other ranges of momenta. This vertex correction is more singular than in the three-dimensional case, due to the factor $(\omega-v_Fq)^{-1}$. Nevertheless, these singularities can be removed by integration, so that they are irrelevant as far as we are interested not in the vertex corrections themselves but rather in other quantities, such as the electron self-energy, etc, which are expressed in terms of Γ by integrals. The denominator $\omega-v_Fq$ would be effective in the phonon spectrum only for $c\approx v_F$, but in the limiting cases $v_F\gg c$ or $v_F\ll c$ this singular factor is associated with virtual phonons. One therefore may say that, due to the presence of the factor $c\sim v_F(m/M)^{1/2}$, the first-order correction to the vertex function is $O(m/M)^{1/2}$.

The lowest-order contribution to the electron self-energy is given by

$$\Sigma_0(\boldsymbol{p})=\mathrm{i}g^2(2\pi)^{-2}\int \mathrm{d}\boldsymbol{p}'G_0(\boldsymbol{p}')D_0(\boldsymbol{p}-\boldsymbol{p}'), \tag{21}$$

which, after performing the integration, becomes

$$\Sigma_0(\boldsymbol{p})=\frac{cg^2}{4\pi}\left\{\frac{2v_F(|p|-k_F)}{v_F^2-c^2}-\frac{\varepsilon-\mu-v_F(|p|-k_F)}{(v_F-c)^2}\ln\left|\frac{\varepsilon-\mu-c(|p|-k_F)}{\varepsilon-\mu-v_F(|p|-k_F)}\right|\right.$$
$$-\frac{\varepsilon-\mu-v_F(|p|-k_F)}{(v_F+c)^2}\ln\left|\frac{\varepsilon-\mu+c(|p|-k_F)+k_c(v_F+c)}{\varepsilon-\mu-v_F(|p|-k_F)}\right|$$
$$\left.\times\frac{\varepsilon-\mu+c(|p|-k_F)-k_c(v_F+c)}{\varepsilon-\mu+c(|p|-k_F)}\right|\Bigg\} \tag{22}$$

for $k_F-k_c<|p|<k_F+k_c$, whence

$$\Sigma_0(\pm k_F,\varepsilon)=-\frac{cg^2}{4\pi}\frac{\varepsilon-\mu}{(v_F+c)^2}\ln\left|1-\frac{(v_F+c)^2k_c^2}{(\varepsilon-\mu)^2}\right|. \tag{23}$$

Singularities in (22) appear only for (i) $|\varepsilon - \mu| > v_F k_c$ and (ii) $\varepsilon - \mu = \pm c(|p| - k_F)$. As long as we are interested in those values of ε which are in the range $\mu - v_F k_c < \varepsilon < \mu + v_F k_c$ singularities of type (i) are not important. For the non-interacting system $\varepsilon - \mu = v_F(|p| - k_F)$. Assuming that the interaction does not change appreciably these energies it results that singularities of type (ii) are also unimportant in the limiting cases $v_F \gg c$ or $v_F \ll c$. Under these circumstances one may say that $\Sigma_0(\boldsymbol{p})$ is $O(m/M)^{1/2}$. From (23) $\Sigma_0(\pm k_F, \mu) = 0$; therefore, we can conclude that, unlike the three-dimensional case, the forward scattering does not shift the Fermi level within the lowest-order approximation of $\Sigma(\boldsymbol{p})$. Moreover, as it results from (23), there is no electron dressing in the order $(m/M)^{1/2}$. This result is consistent with that given by (18*b*).

Making use of the lowest-order expression of the electron self-energy, the Ward identity (11) reads

$$\Gamma^f_{\pm}(\boldsymbol{p}, \boldsymbol{q}) = g\left(1 - \frac{\Sigma_{0\pm}(\boldsymbol{p}) - \Sigma_{0\pm}(\boldsymbol{p} - \boldsymbol{q})}{\omega \mp v_F q}\right). \tag{24}$$

As $\Sigma_0(\boldsymbol{p})$ is $O(m/M)^{1/2}$ and the singular denominator is ineffective we conclude that the renormalised vertex function given by (24) may be taken of the form $\Gamma^f_{\pm} = g[1 + O(m/M)^{1/2}]$, in agreement with the Migdal theorem.

4. Backscattering and Kohn anomaly

Introducing the Ward identity for the backscattering processes (12) into (13) we obtain, as in the forward scattering case, the irreducible polarisation

$$\Pi^b_{\pm}(\boldsymbol{q}) = \begin{cases} -\dfrac{\lambda}{2} \ln \left| \dfrac{\omega^2 - v_F^2(2k_c - |q|)^2}{\omega^2 - v_F^2 q^2} \right| & 0 < |q| < k_c, \\ 0 & k_c < |q| < 2k_c, \end{cases} \tag{25}$$

where the + (−) sign refers to $p \sim +k_F$ ($-k_F$) and momentum transfer $2k_F + q$ ($-2k_F - q$). The phonon Green function and the electron-density correlation function with momentum transfer $2k_F (q = 0)$ possess the same type of singularities as the four-point vertex function does in the case of electron–electron interaction within the logarithmic approximation (Sólyom 1979). The effect of these singularities on the phonon spectrum around $2k_F$ will be discussed below.

The normal modes for the backscattering interaction are given by

$$\frac{\Omega_q^2}{\omega_0^2} - 1 = -\frac{\lambda}{2} \ln \left| \frac{\Omega_q^2 - v_F^2(2k_c - |q|)^2}{\Omega_q^2 - v_F^2 q^2} \right|, \qquad 0 < |q| < k_c, \tag{26}$$

where ω_0 has been taken for the bare phonon frequency at wavevectors near $2k_F$, $\omega_0 = \omega_{2k_F + q}$. We are interested only in those solutions of (26) which correspond to dressed phonons. As it can be seen from (26) the phonon frequency becomes imaginary at wavevectors in the range $\pm 2k_F - q_{SM} < \pm 2k_F + q < \pm 2k_F + q_{SM}$, where $q_{SM} = 2k_c(1 + e^{1/\lambda})^{-1} < k_c$. This soft mode, arising in the phonon spectrum, points out an instability of the system against the backscattering interaction. This instability is similar to that occurring in the one-dimensional electron system with attractive backscattering interaction (Apostol 1981b). The softening of the phonon modes is an indication of the breaking down of the perturbation theoretical approach. This is why we are prevented from discussing the Migdal theorem for the backscattering interaction within this approx-

imation. Our aim here is to discuss the dispersion relation of the longitudinal acoustical phonons near the $2k_F$ anomaly observed in KCP ($K_2Pt(CN)_4Br_{0.3} \cdot 3.2D_2O$).

It is well known that previous x-ray diffuse-scattering experiments (Comès *et al* 1973a, b) performed at room temperature on KCP revealed the existence of a superstructure of period $6d_\parallel$($d_\parallel = 2.89$ Å is the Pt–Pt distance along the chain) which corresponds to the $2k_F$ scattering ($k_F = 0.85 \times 2\pi/c$, $c = 2d_\parallel$ is the lattice constant along the chain direction). Unfortunately, this type of experiment could not resolve whether the $2k_F$ scattering was elastic or inelastic, i.e., whether the distortion results from a Peierls instability (static distortion) or a giant Kohn anomaly (dynamic distortion). Electrical conductivity (see, for example, Shchegolev 1972), thermopower (Kuse and Zeller 1972) and nuclear magnetic resonance (Niedoba 1979) measurements show that below 100 K a static Peierls distortion is responsible for the band semiconductor behaviour of KCP. Lynn *et al* (1975) claimed that at all temperatures below 300 K the Pt–Pt distances are subject to a $2k_F$ sinusoidal distortion along the chain caused by the electronic charge-density wave (CDW). The correlation length along the chain is more than 100 $d_\parallel$, whereas the different chains are weakly correlated, at least at temperatures above 100 K, as described by a transverse correlation length of 6 Å (the interchain distance is about 9.87 Å). On the other hand, Kuse and Zeller (1971) measured the optical reflectivity of KCP at high temperatures for light polarised parallel to the chains and found a reflectivity which is characteristic of a metal. Moreover, the neutron inelastic experiments carried out by Renker *et al* (1973, 1974) showed that in addition to the elastic scattering a contribution from a giant Kohn anomaly is always present at room temperature in the $2k_F$ scattering, and the transition to a three-dimensional long-range order perpendicular to the Pt chains is never accomplished. Comès *et al* (1975) concluded that only at high temperatures the phonon spectrum is strongly distorted whereas a low temperature the Kohn anomaly has almost vanished. A resonance was found by these authors at approximately 2.5 meV which was interpreted by them as a low-lying optical mode. From these experimental data one arrives at the picture of KCP as being a one-dimensional conductor which exhibits a giant Kohn anomaly at room temperature and a Peierls insulator at low temperatures. A static $2k_F$ distortion along the chains is probably present at all temperatures, strongly fluctuating at high temperature and more distinct and correlated in the direction perpendicular to the chains below 100K. A microscopic theory was attempted by Rice and Strässler (1973) which shows explicitly how the giant Kohn anomaly can be the precursor of the Peierls distortion with decreasing temperature.

This overall picture of KCP was further specified by Carneiro *et al*(1976), who investigated the lattice dynamics by inelastic neutron scattering experiments. We shall summarise here the results of these authors. The lattice dynamics of KCP is strongly anisotropic—the phonons propagating along the c^* direction having much higher frequencies than those propagating in the basal plane of the Brillouin zone. The dispersion relations have been measured for the longitudinal acoustical phonons propagating with wavevectors $(0, 0, \zeta)$ (Λ branch) and $(\frac{1}{2}, \frac{1}{2}, \zeta)$ (V branch), ζ being the component parallel to the c^* axis. A giant Kohn anomaly has been found at all temperatures between 20 K and 240 K for $\zeta = 0.3c^*$ which corresponds to the $2k_F$ scattering. The inelastic scattering intensities are found to vary slowly with the wavevector component perpendicular to the chains and do not reflect the build-up of the transverse correlations at lower temperatures. The temperature dependence was found to be rather small, indicating that the phonon–phonon interaction is not very important. A longitudinal optic phonon has been measured at 6 meV in agreement with the Raman scattering data reported by Steigmeier *et al* (1975). A maximum in the $2k_F$ scattering was found at all temperatures

below 160 K with an energy of 2.5 meV. This value agrees fairly well with that of 1.9 meV obtained by Brüesch *et al* (1975) from IR reflectivity measurements. The inelastic scattering is separated in energy from the elastic scattering at lower temperatures. The apparent disappearance of this phonon gap at higher temperatures is ascribed to phonon lifetime effects, so that the phonon frequency does not condense to zero at any temperature. The scattering at the $2k_F$ anomaly does not present any wavevector extension below 4.5 meV, in contrast to the results obtained by Comès *et al* (1975). The excitations responsible for this scattering are at all temperatures connected with the regular phonons, whose frequency is $\omega_0 = 8$ meV in the neighbourhood of the $2k_F$ anomaly. Carneiro *et al* (1976) used a simple model for the dispersion relation of the distorted phonons in the vicinity of $2k_F$ to analyse the neutron scattering intensities below $\omega_M = 4.25$ meV. Their model has a linear part which is cut off by a flat part of frequency ω_T. In the (q, ω) plane the linear part decreases from the point (q_M, ω_M) to the point (q_T, ω_T). These parameters vary slowly with temperature. Their values, deduced from the data given by Carneiro *et al* (1976), are given in table 1. As was emphasised by these authors the excitations measured in the $2k_F$ anomaly cannot be consistently analysed within the framework of the CDW model (Lee *et al* 1974). Whereas the high-lying optical mode of 6 meV can be associated with the amplitude mode of the CDW the attempt to associate the low-lying mode of 2.5 meV with the phason excitations of the CDW leads to inconsistent results. In connection with this we should emphasise that the transition to a well-defined distorted Peierls state, as it is predicted by the mean-field theory of the

Table 1. Values of the parameters q_M, q_T, ω_T derived from the data given by Carneiro *et al* (1976) ($\omega_0 = 8$ meV. $\omega_M = 4.25$ meV, $v_F = 11 \times 10^5$ m s^{-1}. $k_F = 0.93$ Å^{-1}) and $k_c\lambda$ obtained from (30).

T (K)	q_M (10^{-3} Å^{-1})	q_T (10^{-3} Å^{-1})	ω_T (meV)	k_c (10^{-3} Å^{-1})	λ
40	2.2	1	2.62	25	0.22
60	2.26	1	2.58	10	0.32
80	3.12	1.5	2.65	15	0.31
100	4.6	2.5	2.71	35	0.25
120	5.1	3	2.84	30	0.27
140	7.17	5	2.96	102	0.20
160	7.86	5.5	3.16	140	0.19

CDW model, is never fully accomplished (Brüesch *et al* 1975). Consequently, it seems more apropriate to describe the excitations with wavevectors near $2k_F$ as being distorted phonons of a giant Kohn anomaly. This is the task we assume in the remainder of this paper. As the frequency of the longitudinal acoustical phonons is weakly dependent on the transverse component of the wavevector we expect our strictly one-dimensional model to work satisfactorily well.

The irreducible polarisation can be calculated straightforwardly at finite temperature, so that the frequency of the dressed phonons is given by

$$\frac{\Omega_q^2}{\omega_0^2} - 1 = \lambda \int_{-1+|q|/2k_c}^{1-|q|/2k_c} dx \frac{1}{2x - \Omega_q/v_F k_c} \left(\frac{1}{1 + \exp[\delta(x + q/2k_c)]} - \frac{1}{1 + \exp[\delta(-x + q/2k_c)]} \right) \qquad 0 < |q| < 2k_c, \tag{27}$$

where $\delta = v_F k_c / k_B T$. The soft mode is present below a critical temperature T_0 which is obtained from (27) by requiring the phonon frequency be zero at $2k_F(q = 0)$:

$$1 = \lambda \int_0^{\delta_0/2} dx \frac{\tanh x}{x}, \qquad \delta_0 = v_F k_c / k_B T_0. \tag{28}$$

There always exists a critical temperature T_0 which satisfies (28) for any λ. For $\delta_0 \gg 1$ (which means λ less than unity) we get

$$k_B T_0 \cong 1.13 v_F k_c \, e^{-1/\lambda}. \tag{29}$$

A condition similar to (29) has been discussed by Berlinsky (1979). However in the present approach we allow for an explicit dependence of the cut-off parameter k_c, much smaller than the Fermi momentum. The presence of this parameter ensures the existence of the renormalised phonons down to lower temperatures. It will be shown that it is the same parameter which also governs the width of the anomalous dip at the frequency of the regular phonons. It appears that the parameter k_c is an essential ingredient of our theory of the Kohn anomaly. Numerical calculations show that the integral in the RHS of (27) does not in practice depend on Ω_q for small values of $\Omega_q / v_F k_c$. Therefore we may neglect this quantity in the denominator of the integrand of (27). In order to fit the curves given by Carneiro *et al* (1976) we impose our Ω_q given by (27) to pass through the points of coordinates $(0, \omega_T)$ and (q_M, ω_M). These requirements read

$$\begin{aligned} \frac{1}{\lambda}\left(1 - \frac{\omega_T^2}{\omega_0^2}\right) &= \int_0^{\delta} \frac{dx}{x} \frac{\sinh x}{1 + \cosh x}, \\ \frac{1}{\lambda}\left(1 - \frac{\omega_M^2}{\omega_0^2}\right) &= \int_0^{\delta(1-\beta_M)} \frac{dx}{x} \frac{\sinh x}{\cosh \delta\beta_M + \cosh x} \end{aligned} \tag{30}$$

where $\beta_M = q_M / 2k_c$. Dividing these equations to one another we obtain an expression independent of λ which provides us with the condition for k_c. Taking the values for ω_T, ω_M and q_M from table 1 and using $v_F = 11 \times 10^5$ m s^{-1} and $\omega_0 = 8$ meV we are able to

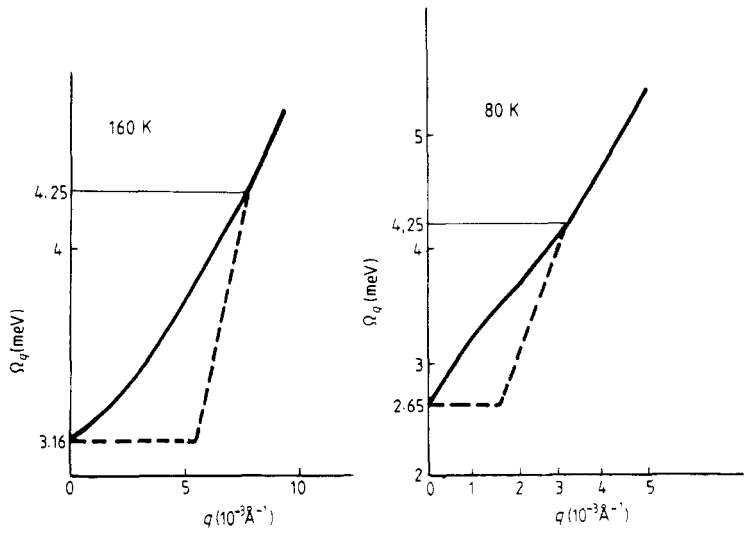

Figure 2. Phonon frequency Ω_q given by (27) (full curve) and by Carneiro *et al* (1976) (broken curve) around $2k_F$ ($q = 0$) at $T = 80$ K and 160 K. The parameters are given in table 1.

calculate numerically the values of the parameter k_c at various temperatures. Having known k_c we can easily derived the value of the coupling constant λ from (30). These values of k_c and λ are given in table 1. The phonon frequency Ω_q given by (27) is plotted versus q in figure 2 (full curve) at $T = 80\,\mathrm{K}$ and $160\,\mathrm{K}$ together with the curves given by Carneiro *et al* (1976) (broken curves). One can see from table 1 that the values of the parameter k_c are much smaller than the Fermi momentum $k_F = 0.93\ \text{Å}^{-1}$. Introducing the values of λ and k_c in (29) we get an upper limit for T_0 of $0.6\,\mathrm{K}$, a value much lower than any temperature at which we performed the calculations. This proves the consistency of our calculations.

One can see from figure 2 that our dispersion relation Ω_q satisfactorily reproduces the curves given by Carneiro *et al* (1976) except for the flat bottom. This flat bottom is due to a finite lifetime of the phonons and we expect that our model might account for it when the lifetime effects would be included.

Recently, Nielsen and Carneiro (1980) obtained for the electron–phonon coupling constant λ the value of 0.3, within the framework of the mean-field theory of the CDW model†. One can see from table 1 that our values for λ are in good agreement with this value at temperatures between $120\,\mathrm{K}$ and $60\,\mathrm{K}$, except for the value 0.25 corresponding to $T = 100\,\mathrm{K}$. A more detailed investigation would be required at this point, in order to take into account the structural changes undergone by the system around this temperature. We expect the CDW model to be valid in this intermediate range of temperature ($120\,\mathrm{K}$–$60\,\mathrm{K}$) since the large fluctuations from the high-temperature region begin to be progressively correlated by the interchain interaction with decreasing temperature. The disagreement between $\lambda = 0.2$ at high temperatures obtained by us and $\lambda = 0.3$ predicted by the mean-field theory of the Peierls transition originates in the presence of the large fluctuations and the pseudo-gap (Brüesch *et al* 1975) which are neglected in the mean-field theory of the CDW. At lower temperatures ($T \lesssim 40\,\mathrm{K}$) the pinning of the CDW becomes more effective and we expect again the mean-field theory of the CDW to be inappropriate for the real situation. In this temperature region our model should also be improved to take into account the effects of the impurities which might cause the pinning of the CDW. At all temperatures our model should be corrected for the $2k_F$ distortion of the lattice by allowing a variation of the overlap integral with the ion–ion distance along the chain (Bjeliš *et al* 1974). This leads to the investigation of the interplay between the elastic and inelastic components in the neutron scattering, as was attempted by Dieterich (1975) by using the dynamic structure factor. A direct comparison of this type of calculation with the intensity contours given by Carneiro *et al* (1976) for the neutron inelastic scattering in the $2k_F$ anomaly of KCP would be most desirable.

5. Conclusions

We have studied the one-dimensional electron–phonon coupling within the perturbation theoretical approach. The Ward identity has been derived for the forward scattering and generalised to the backscattering by assuming that the interaction does not distort appreciably the Fermi sea (weak-coupling limit). In the case of the forward scattering it has been shown that the corrections to the zeroth-order value of the electron–phonon vertex are $O(m/M)^{1/2}$ in agreement with the Migdal theorem. A model has been proposed

† This value seems to be more reliable than other estimates, such as $\lambda = 0.192$ (Carneiro *et al* 1979) and $\lambda = 0.21$–0.24 (see, for example, Berlinsky 1979), all of these being derived from approximate equations of the CDW theory.

for the backscattering interaction having explicitly introduced the cut-off parameter k_c. It has been shown that this parameter can be related in a simple way to the Kohn anomaly observed in the phonon spectrum around $2k_F$. The strong distortion near $2k_F$ reported by Carneiro *et al* (1976) for the longitudinal acoustical phonons in KCP has been fitted by our theoretical calculations and the electron–phonon coupling constant has been derived. We found good agreement of our values for λ with those predicted by the CDW model.

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