Sound propagation in density wave conductors and the effect of long-range Coulomb interaction

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(December 31, 2021)

Abstract

We study theoretically the sound propagation in charge- and spin-density waves in the hydrodynamic regime. First, making use of the method of co-moving frame, we construct the stress tensor appropriate for quasi-one dimensional systems within tight-binding approximation. Taking into account the screening effect of the long-range Coulomb interaction, we find that the increase of the sound velocity below the critical temperature is about two orders of magnitude less for longitudinal sound than for transverse one. It is shown that only the transverse sound wave with displacement vector parallel to the chain direction couples to the phason of the density wave, therefore we expect significant electromechanical effect only in this case.

72.15.Nj, 71.45.Lr, 75.30.Fv
I. INTRODUCTION

Several aspects of the collective transport associated with the phason in charge- or spin-density waves (CDW or SDW) are still not well understood. One of the intriguing phenomena is the electromechanical effect observed in CDW [1–3] and more recently in SDW [4]. First of all, most of the elastic moduli increase upon entrance into the CDW or SDW state, often with a sharp dip at $T_c$, the transition temperature. Second, some of the elastic moduli in CDW or SDW soften when the density wave is depinned by an external electric field in excess of the depinning threshold field $E_T$. Third, the change in the elastic moduli due to depinning of the density wave depends on the frequency $\omega$ of the flexural vibration [7], and decreases like $\omega^{-p}$ with $p \approx 1$. This behavior is similar to the frequency dependence of the change in the dielectric constant upon depinning in CDW and SDW [8].

We have shown earlier [9] in the collisionless limit that the hardening of the elastic constants can be understood in terms of the reduction in the quasiparticle screening of the ion potential due to the formation of the density wave state. The electromechanical effect was interpreted as an additional screening contribution from the collective mode of the density wave condensate (phason) liberated by depinning. A later extension of that theory to the experimentally more relevant hydrodynamic limit [10] did not modify the above picture qualitatively. However in these papers it was assumed that the phonon simply couples to the electronic density, and the effect of the long-range Coulomb interaction was neglected.

The purpose of the present paper is twofold. First, we shall develop the theory of the electron-phonon coupling for a strongly anisotropic system, which will enable us to distinguish between the behavior of transverse and longitudinal sound waves propagating in various directions. Second, we shall include the effect of the long-range Coulomb interaction following Kadanoff and Falko [11]. In Section II we construct the electronic stress tensor (which couples to the deformation tensor of the sound wave) for a quasi-one dimensional system following the method of comoving frame [12]. In Section III we concentrate on
the quasiparticle contribution to the stress tensor correlation functions corresponding to
the pinned case. Section IV is devoted to the examination of the coupling of the stress
tensor to the phason, which is relevant to the electromechanical effect. Our conclusions are
summarized in Section V. A preliminary report on this work has already been published
elsewhere [13].

II. ELECTRON-PHONON COUPLING

Following Tsuneto [12] let us assume that both the ionic potential and the electronic
wavefunction are deformed in the slowly varying sound field \( u(r, t) = u \cos(qr - \omega t) \) imposed
externally (extreme tight-binding limit):

\[
\begin{align*}
V(r) &\rightarrow V[r - u(r, t)] \\
\psi(r) &\rightarrow \psi[r - u(r, t)](1 + \nabla u)^{-1/2}.
\end{align*}
\]

This displacement is generated by the unitary operator \( U = \exp[-u(r, t)\nabla] \). Therefore the
deformed wavefunction is an eigenfunction of the transformed Hamiltonian \( h = Uh_0U^+ \),
where \( h_0 = \varepsilon(-i\nabla) \) with \( \varepsilon(p) \) being the zone-periodic electronic energy spectrum. The
transformed Hamiltonian \( h \) is then expanded in terms of the deformation tensor \( \nabla_i u_j \), which
is much smaller than one, even though the displacement \( u \) itself may be many times of the
lattice constant for sound propagation. We obtain \( h = h_0 + h_{el-ph} \), where the Hamiltonian
for the electron-phonon coupling is given by

\[
h_{el-ph} = \sum_{i,j} (\nabla_i u_j)i\nabla_j v_i(-i\nabla),
\]

with \( v(p) = \partial \varepsilon(p) / \partial p \), the velocity of the Bloch electron. The matrix element of \( h_{el-ph} \)
between Bloch states is evaluated as

\[
\langle p + q | h_{el-ph} | p \rangle = -i \sum_{i,j} q_j u_i \tau_{ij}(p),
\]

where the stress tensor
\[
\tau_{ij}(p) = mv_i(p)v_j(p),
\]  
and \(m\) is the bare electron mass. This expression generalizes the stress tensor used for an isotropic metal \[\text{[11]}\].

In orthorombic symmetry the sound wave polarized in the \(i\) direction and propagating in the \(j\) direction couples to the \(\tau_{ij}\) component of the stress tensor, and in order to determine the effect of that coupling on the frequency (or velocity) of the sound, we have to evaluate the appropriate stress tensor correlation function \(\langle [\tau_{ij}, \tau_{ij}] \rangle\). Once this is known, the renormalized sound velocity can be calculated in the weak coupling limit as

\[
c = c_0 \{1 - \langle [\tau, \tau] \rangle / 2M c_0^2\},
\]

where \(c_0\) is the sound velocity without electron-phonon coupling, \(M\) is the ion mass, and for clarity we have suppressed the indices both for the stress tensor component and for the sound velocity.

For a highly anisotropic \((t_a \gg t_b \gg t_c)\) tight-binding dispersion

\[
\varepsilon(p) = -2t_a \cos(ap_x) - 2t_b \cos(bp_y) - 2t_c \cos(cp_z) - \mu,
\]

widely used for CDW and SDW materials \[\text{[14]}\], the velocity and stress tensor components are easily obtained, and their values on the open Fermi surface can conveniently be expressed by the component of \(p\) perpendicular to the chains (\(x\) direction). However, since the Green’s functions for CDW and SDW are usually written in the left-right spinor representation \[\text{[10]}\], involving measuring momenta from \(\pm Q/2\) with the density wave wavevector \(Q = (2p_F, \pi/b, \pi/c)\), we should express the stress tensor elements in a compatible manner. It turns out, that for each stress tensor component the term proportional to the unit matrix dominates, therefore we have

\[
\begin{align*}
\tau_{xx} &= mv_y^2 \{1 - [t_b/t_a \sin(ap_F)]^2 \sin^2(bp_y)\} \\
\tau_{yy} &= mv_y^2 [1 + \cos(2bp_y)] \\
\tau_{xy} &= mv_F v_y \sqrt{2} \cos(bp_y).
\end{align*}
\]
Here $p_F$ is the Fermi momentum, $v_F = 2at_a \sin(ap_F)$ is the Fermi velocity in the chain direction, while $v_y = \sqrt{2bt_b} \ll v_F$ is a typical velocity in the perpendicular direction. In the followings we restrict our study to the $x-y$ plane, since behavior involving the $z$ direction should be similar to that of the $y$ direction. We note, that all components of the stress tensor depend on momentum through the combination $\varphi = bp_y$ only.

III. PINNED DENSITY WAVES

In this section we consider sound propagation with no applied electric field. The density wave is pinned, therefore the condensate is unable to contribute to correlation functions, including that for the stress tensor. Mathematically this situation can be simulated by setting the coupling of the stress tensor (and of the density) to the phason to zero. Then the stress tensor couples only to the density fluctuations, resulting in the well known Coulomb screening [11]:

$$\langle [\tau, \tau] \rangle = \langle [\tau, \tau] \rangle_0 - \frac{\langle [\tau, n] \rangle_0 \langle [n, \tau] \rangle_0}{q^2/4\pi e^2 + \langle [n, n] \rangle_0}. \tag{8}$$

Here $n$ stands for the electronic particle density, and $\langle [A, B] \rangle_0$ denotes a correlation function, in which only the effect of impurity scattering is taken into account.

The density correlator $\langle [n, n] \rangle_0$ in the presence of impurity scattering was evaluated in [10]. A straightforward extension of that calculation confirms that under the circumstances of the sound experiment ($lq \ll 1$, where $l$ is the mean free path) the stress tensor correlator has two distinct contributions:

$$\langle [\tau, \tau] \rangle_0 = \langle \tau(\varphi) \rangle^2_\varphi \langle [n, n] \rangle_0 + \langle (\delta \tau(\varphi))^2 \rangle_\varphi \langle [n, n] \rangle_0^{\text{novertex}}. \tag{9}$$

The first contribution features only the average of the stress tensor $\langle \tau(\varphi) \rangle_\varphi = (2\pi)^{-1} \int_{-\pi}^{\pi} d\varphi \tau(\varphi)$, and is proportional to the diffusive (vertex corrected) density correlator. The second contribution contains only the fluctuating part of the stress tensor component $\delta \tau(\varphi) = \tau(\varphi) - \langle \tau(\varphi) \rangle_\varphi$, and therefore it is proportional to the density correlator.
\[\langle [n,n]\rangle_0^{novertex}\] calculated without vertex corrections. According to the same argument, only the average of the stress tensor couples to the density, therefore

\[\langle [\tau,n]\rangle_0 = \langle [n,\tau]\rangle_0 = \langle \tau(\varphi)\rangle \langle [n,n]\rangle_0.\] (10)

Combining Eqs.(8)-(10) we see that in the long wavelength limit appropriate for the sound experiment \((q \approx 1/L,\) where \(L\) is the sample size), the average part of the stress tensor \((s\text{-wave component, proportional to density})\) is completely screened out by the Coulomb interaction, and only the fluctuating part contributes to the correlation function:

\[\langle [\tau,\tau]\rangle = \langle [\delta \tau(\varphi)]^2 \varphi \langle [n,n]\rangle_0^{novertex}.\] (11)

The situation here is the same as in the electronic Raman scattering, where the long-range Coulomb interaction suppresses the density (charge) fluctuations, and only non-\(s\)-wave channels survive \([15]\).

The evaluation of \(\langle [n,n]\rangle_0^{novertex}\) can be done starting with the results of \([10]\). The calculation is rather technical, therefore we delegate it to the Appendix, and we give here the results only. Without vertex corrections there is no diffusion pole, and both the wavenumber \(q\) and the frequency \(\omega\) could be set to zero. However we keep a finite (but small) frequency for finite imaginary part of the correlator:

\[\langle [n,n]\rangle_0^{novertex} = N_F \frac{i\tilde{\Gamma}_{qp}(1 - \tilde{f})}{\omega + i\tilde{\Gamma}_{qp}},\] (12)

where \(N_F\) is the density of states at the Fermi surface. The corresponding "unrenormalized" condensate density \(\tilde{f}\) (for the general formula see Eq.(32) in the Appendix) and quasiparticle damping \(\tilde{\Gamma}_{qp}\) are evaluated in two limiting cases, close to \(T_c\) and close to zero temperature as

\[\tilde{f}(T \to T_c) = -2(\frac{\Delta}{4\pi T})^2\psi''(\frac{1}{2} + \frac{\Gamma}{2\pi T}) \approx 7\zeta(3)(\frac{\Delta}{2\pi T})^2\]

\[\tilde{f}(T \to 0) = 1 - 3\pi\alpha/16,\] (13)

and
\[
\tilde{\Gamma}_{qp}(T \rightarrow T_c) = 2\Gamma
\]
\[
\tilde{\Gamma}_{qp}(T \rightarrow 0) = \left(\frac{9\pi}{32} u_0^2/15 - 4\alpha^2/3 \right) G/T e^{G/T}.
\]

Here \(\Delta\) is the density wave order parameter, \(\Gamma = \Gamma_F + \Gamma_B/2\) is a combination of the impurity forward and backscattering rate, \(\alpha = \Gamma/\Delta\), \(u_0^2 = 1 - \alpha^2/3\) and \(G = \Delta u_0^2\) is the density wave gap.

As it is seen from Eq.(13), \(\tilde{f}\) increases linearly in \((T_c - T)\) below \(T_c\), but it is slightly less than one at \(T = 0\) (\(\Gamma\) is usually an order of magnitude smaller than \(T_c\)). Nevertheless, the temperature dependence of the sound velocity in the pinned case will still be qualitatively the same as in the collisionless limit \([I]\). The relative change of the sound velocity compared to the normal state \((c_n)\) is easily obtained from Eqs.(5), (11) and (12) as

\[
\frac{(c - c_n)}{c_0} = \lambda \tilde{f},
\]

where the effective coupling

\[
\lambda = \frac{N_F}{2Mc_0^2} \langle [\delta \tau(\varphi)]^2 \rangle_{\varphi}.
\]

Using Eq.(7), these effective couplings for the various sound waves are

\[
\lambda_{xx} = \frac{N_F(mv_x^2)}{16Mc_0^2} \left( \frac{t_b}{t_a \sin(\alpha_F)} \right)^4
\]
\[
\lambda_{yy} = \frac{N_F(mv_y^2)}{4Mc_0^2}
\]
\[
\lambda_{xy} = \frac{N_F(mv_yv_x)}{2Mc_0^2}.
\]

Since \(v_y/v_F \approx t_b/t_a \approx 1/10\) in many quasi one dimensional materials, we expect that the relative increase of the sound velocity below \(T_c\) will be a factor \(10^2\) smaller for longitudinal sound than for transverse sound.

**IV. ELECTROMECHANICAL EFFECT**

If an external electric field in excess of the threshold field \(E_T\) of the nonlinear conductivity is applied in the chain direction, then the condensate is depinned and is able to contribute
to various correlation functions \[9\]. The best known example is of course the conductivity itself, but the situation is the same for the stress tensor correlator as well. The collective contribution to \(\langle [\tau, \tau] \rangle\) can be obtained if we allow both the stress tensor and the density to couple to the phason (in the previous section this coupling was blocked due to pinning). In this case the stress tensor correlator has another contribution \(\langle [\tau, \tau] \rangle_{\text{coll}}\) in addition to the one calculated in the previous section, namely:

\[
\langle [\tau, \tau] \rangle_{\text{coll}} = \frac{U\langle [\tau, \delta\Delta] \rangle_{\text{Coul}}\langle [\delta\Delta, \tau] \rangle_{\text{Coul}}}{1 - U\langle [\delta\Delta, \delta\Delta] \rangle_{\text{Coul}}}. \tag{18}
\]

Here \(U\) is the on-site Coulomb repulsion responsible for the formation of the SDW state (for CDW it should be replaced by the phonon propagator, but that does not affect our conclusions), \(\delta\Delta\) is the phase fluctuation of the order parameter, and \(\langle [A, B] \rangle_{\text{Coul}}\) is the correlation function of quantities \(A\) and \(B\) including the effect of the long-range Coulomb interaction (like in Eq.(8)). As we have seen earlier, in the long wavelength limit this yields:

\[
\langle [A, B] \rangle_{\text{Coul}} = \langle [A, B] \rangle_0 - \langle [A, n] \rangle_0\langle [n, B] \rangle_0/\langle [n, n] \rangle_0. \tag{19}
\]

First we consider if the allowed coupling to the phason actually takes place for various sound waves. According to Eq.(18) we need to examine \(\langle [\tau, \delta\Delta] \rangle_{\text{Coul}}\), which is given by Eqs.(19) and (10) as

\[
\langle [\tau, \delta\Delta] \rangle_{\text{Coul}} = \langle [\tau, \delta\Delta] \rangle_0 - \langle \tau(\varphi) \rangle_\varphi\langle [n, \delta\Delta] \rangle_0. \tag{20}
\]

The density-phason correlator \(\langle [n, \delta\Delta] \rangle_0\) was evaluated in \[10\]. Here we only reiterate that result in the limit of experimental interest \(lq \ll c_0/v_F\) (dynamic limit):

\[
\langle [n, \delta\Delta] \rangle_0 = iN_F\frac{\zeta(\varphi)}{2\Delta}f_d, \tag{21}
\]

where in our two dimensional geometry the wavenumber \(q\) appears in \(\zeta(\varphi) = v_Fq_x + \sqrt{2}v_yq_y\cos\varphi\), and the condensate density in the dynamic limit is given by:

\[
f_d(T \to T_c) = \frac{\Delta^2}{2\pi T_B} \psi'(\frac{1}{2} + \frac{k}{2\pi T}) \approx \frac{\pi \Delta^2}{4 T_B},
\]

\[
f_d(T \to 0) = 1. \tag{22}
\]
We recall that the same $f_d$ appears in the current-phason correlator $\langle [j, \delta \Delta] \rangle_0$, as well as in the phason propagator [10]. Note that $f_d$ increases from zero much faster below $T_c$ than $\tilde{f}$ does, and that at zero temperature it saturates exactly to 1. The stress tensor-phason correlator can be calculated similarly:

$$\langle [\tau, \delta \Delta] \rangle_0 = iN_F \frac{\langle \tau(\varphi)\zeta(\varphi) \rangle_0}{2\Delta} f_d. \quad (23)$$

Now we shall examine Eq.(20) for different sound waves in order to determine if there is a collective contribution to the corresponding stress tensor correlator. We consider longitudinal and transverse sound waves propagating in the $x$ and $y$ directions. Clearly, the second (screening) term in Eq.(20) is nonzero only for the longitudinal sound propagating in the chain direction ($q \parallel u \parallel x$), in which case it completely cancels the first term, leading to no collective contribution. The other longitudinal sound propagating perpendicular to the chains ($q \parallel u \parallel y$) does not couple to the phason either, because $\langle \tau_{yy}(\varphi) \cos \varphi \rangle_0 = 0$ (see Eq.(7)). The coupling of the transverse wave propagating in the chain direction ($q \parallel x$ and $u \parallel y$) is controlled by $\langle \tau_{xy}(\varphi) \rangle_0 = 0$, yielding again no collective contribution. This means that in all of the above three cases there will be no electromechanical effect.

For the rest of this section we will concentrate on the only interesting case, when the transverse sound propagates perpendicular to the chains ($q \parallel y$ and $u \parallel x$). In this case there will be coupling to the phason, since

$$\langle [\tau_{xy}, \delta \Delta] \rangle_{Coul} = \langle [\tau_{xy}, \delta \Delta] \rangle_0 = iN_F \frac{f_d}{2\Delta} mv_F v_y q_y \quad (24)$$

is nonzero. Now we have to consider the denominator in Eq.(18). Since $\langle [n, \delta \Delta] \rangle_0 = 0$ for $q_x = 0$, therefore $\langle [\delta \Delta, \delta \Delta] \rangle_{Coul} = \langle [\delta \Delta, \delta \Delta] \rangle_0$, and we can use the result for the phason propagator calculated in [10], which in our case reduces to

$$1 - U \langle [\delta \Delta, \delta \Delta] \rangle_0 = \frac{UN_F f_d}{(2\Delta)^2} [(v_y q_y)^2 - i \omega \Gamma_{ph}]. \quad (25)$$

Here $\Gamma_{ph}$ is the phason damping rate and is given by

$$\Gamma_{ph}(T \to T_c) = 2 \Gamma_B$$

$$\Gamma_{ph}(T \to 0) = \frac{8n^2 T_B}{3\alpha_0^2 \pi G} e^{-G/T}. \quad (26)$$
The phason damping freezes out for low temperature, and approaches $2\Gamma_B$ at $T_c$. Note the discontinuity in $\Gamma_{ph}$ at $T_c$ (approaching from above $\Gamma_{ph} \approx 2\pi^3 T/7\zeta(3)$), which is the consequence of the finite order parameter $\Delta$ below $T_c$ exceeding almost immediately the energy scale set by $\omega$ and $vq$.

We are now able to write down the total correlation function for this sound wave in the unpinned case. Using Eqs. (11), (18), (24) and (25) we obtain

$$\langle [\tau_{xy}, \tau_{xy}] \rangle = N_F(mv_Fv_y)^2 \times$$

$$\times \left[ \frac{i\Gamma_{qp}(1-\tilde{f})}{\omega + i\Gamma_{qp}} + \frac{(v_yq_y)^2f_d}{(v_yq_y)^2-\omega^2\Gamma_{ph}} \right].$$

(27)

The above equation means that the collective contribution (the second term on the right hand side) due to the moving condensate recovers some of the screening of the ion motion lost because of the decrease in the number of quasi particles. In fact, at zero temperature it overcompensates somewhat, since $f_d > \tilde{f}$. Therefore we expect the electromechanical effect for the transverse sound polarized in the chain direction only. According to Eq. (27), close to $T_c$ the electromechanical effect on the sound velocity should be much smaller than the temperature effect, while at low temperatures the softening is somewhat bigger than the hardening was upon cooling. Although the collective contribution in Eq. (27) does have a frequency dependence, it does not appear to describe the suppression of the electromechanical effect when the frequency is increased [7]. This is rather puzzling, although the above results for sound propagation may not translate literally to the flexural experiment.

V. CONCLUSIONS

We have derived for the first time the appropriate stress tensor for quasi-one dimensional electron systems. Under conditions of a sound velocity measurement ($lq \ll 1$) the long-range Coulomb interaction has a simple role to suppress the $s$-wave channel as in the theory of electronic Raman scattering. In highly anisotropic systems like Bechgaard salts the increase of the sound velocity in the density wave state is two orders of magnitude
smaller for longitudinal sound waves than for transverse ones. We also find, that a sound wave with polarization perpendicular to the chain direction can not couple to the phason, because the density wave condensate can only move parallel to the chains. The coupling of the longitudinal sound propagating in the chain direction is screened away by the Coulomb interaction, which leaves us only the transverse sound wave propagating perpendicular to the chains as the one which does couple to the phason, and shows the electromechanical effect.

Recently Britel et al. measured the elastic constant $c_{44}$ of $(Ta_{1-x}Nb_xSe_4)_2I$ at 15MHz in the geometry $u \parallel x$ $[17]$, and found a relative reduction of order $10^{-4}$ in the presence of an electric field approximately $10E_T$. This seems to be consistent with our analysis, although the observed effect appears to be a little too small.

ACKNOWLEDGMENTS

This publication is sponsored by the U.S.-Hungarian Science and Technology Joint Fund in cooperation with the National Science Foundation and the Hungarian Academy of Sciences under Project No. 264/92a, which enabled one of us (A.V.) to enjoy the hospitality of USC. This work is also supported in part by the National Science Foundation under Grant No. DMR92-18317 and by the Hungarian National Research Fund under Grants No. OTKA15552 and T4473.

APPENDIX

We evaluate here the density correlation function $\langle [n,n] \rangle_0$ $^{novertex}$ (Eqs.(12)-(14) in the text). We start with the corresponding thermal product (See $[10]$):

$$\langle [n,n] \rangle_0^{novertex} = N_F [1 - \pi T \sum_n F(iu_n, iu'_n)],$$

(28)

where $N_F$ is the density of states, and $u_n$ and $u'_n$ are related to the Matsubara frequencies $\omega_n$ and $\omega'_n = \omega_{n-\nu}$ by
\[ \omega_n/\Delta = u_n[1 - \alpha(u_n^2 + 1)^{-1/2}], \quad (29) \]

with \( \Delta \) the order parameter, \( \alpha = \Gamma/\Delta \) and \( \Gamma = \Gamma_F + \Gamma_B/2 \) a combination of the impurity forward and backscattering rates. Neglecting vertex corrections in the relevant formulas in [10] leads to:

\[ F(u, u') = \frac{1 + uu'\frac{1}{(1 - u^2)\Gamma + (1 - u^2)\text{Re}\langle(1 - u^2)^{-1/2}\rangle}}{\Delta[(1 - u^2)^{1/2}(1 - u^2)^{1/2})]}, \quad (30) \]

where \( u \) and \( u' \) are analytic continuations of \( iu_n \) and \( iu'_n \), and in the absence of the diffusion pole the wavenumber \( q \) was already set to zero.

While evaluating the correlation function we follow the standard method [18]. Expanding up to linear order in \( \omega \) we obtain

\[ \langle[n, n]\rangle_{0\text{vertex}}^0 = N_F(1 - \tilde{f} + i\omega I), \quad (31) \]

where

\[ \tilde{f} = \frac{\pi T}{\Delta} \sum_n (u_n^2 + 1)^{-3/2}, \quad (32) \]

and

\[ I = \frac{1}{2\Delta} \int_G^{\infty} dE \cosh^{-2}\left(\frac{E}{2T}\right) \times \]

\[ \times \left[\text{Re}(1 - u^2)^{1/2} - \text{Re}(1 - u^2)^{-3/2}\right]. \quad (33) \]

Here \( h' = (1/2)[1 + (|u|^2 + 1)/|u^2 - 1]|, \) and \( G = \Delta u_0^3 \) is the gap with \( u_0^3 = 1 - \alpha^{2/3} \). The above equations can be evaluated in two limiting cases, with temperature close to \( T_c \) and close to zero, and can be brought to the form of Eqs.(12)-(14) in the text.
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