RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 36, NUMBER 5 15 AUGUST 1987-I

Elastic properties of charge-density-wave conductors

Kazumi Maki* and Attila Virosztek†
Max-Planck-Institut für Festkörperforschung, 7000 Stuttgart 80, Federal Republic of Germany
(Received 2 March 1987)

The sound propagation in a charge-density wave (CDW) in quasi-one-dimensional systems is studied theoretically within the mean-field approximation. We find that the sound velocity is unaffected by the CDW transition in the absence of CDW pinning. However, in the presence of CDW pinning the sound velocity increases upon entrance into the CDW state. The present result offers a simple interpretation of the field dependence of Young's modulus observed in a CDW of TaS_3.

The nature of charge-density-wave (CDW) configurations in quasi-one-dimensional conductors is currently being studied rather extensively.[1] Recent elegant experiments by Brill and co-workers[2,3] and by Mozurkewich, Chaikin, Clark, and Grüner[4] show that not only the electronic properties but also the elastic properties depend sensitively on the CDW configuration.

Within a model used by Lee, Rice, and Anderson[5] (LRA) we study the elastic properties of a CDW. As is well known, the longitudinal sound velocity is expressed in terms of the polarization operator $\Pi(q,\omega)$ as[6]

$$c=c_0[1-g^2\Pi(q,0)]^{1/2} \,, \tag{1}$$

where c_0 is the bare sound velocity and g is the electron-phonon coupling constant. Since $\Pi(q,\omega)$ is the density correlation function and the density fluctuation couples to the sliding motion of the CDW, Π ($\equiv\langle[n,n]\rangle$) is given within mean-field theory[5]

$$\langle[n,n]\rangle=\langle[n,n]\rangle_0-g^2D_0(\omega)\frac{\langle[n,\delta\Delta]\rangle_0^2}{1+g^2D_0(\omega)\langle[\delta\Delta,\delta\Delta]\rangle_0} \,, \tag{2}$$

where

$$D_0(\omega)=\omega_Q^2(\omega^2-\omega_Q^2)^{-1} \tag{3}$$

is the bare phonon propagator with momentum $Q=2k_F$ and $\langle\ \rangle_0$ means the thermal average taken when the interaction between fluctuations is neglected. We note that in Eq. (2), $\delta\Delta$ is essentially the component of n with the momentum $\pm Q$. Following LRA[5] we obtain

$$\langle[n,n]\rangle_0(q,\omega)=2N_0[1-(2\Delta)^2F]\zeta^2(\zeta^2-\omega^2)^{-1} \,,$$

$$\langle[n,\delta\Delta]\rangle_0(q,\omega)=2\sqrt{2}N_0\zeta\Delta F \,,$$

and

$$\langle[\delta\Delta,\delta\Delta]\rangle_0(q,\omega)=N_0[1/\lambda-(\zeta^2-\omega^2)F] \,, \tag{4}$$

where F has been defined elsewhere[7]

$$F=(\zeta^2-\omega^2)\int_\Delta^\infty dE(E^2-\Delta^2)^{-1/2}\tanh(\tfrac{1}{2}\beta E)\frac{N}{D} \,,$$

$$N=(\zeta^2-\omega^2)^2-4E^2(\omega^2+\zeta^2)+4\Delta^2\zeta^2 \,, \tag{5}$$

$$D=N^2-64E^2\zeta^2\omega^2(E^2-\Delta^2) \,,$$

and $\lambda=g^2N_0$, $\zeta=vq$, v is the Fermi velocity, and q is the momentum parallel to the chain direction. Substituting Eq. (4) into Eq. (2) we obtain

$$\Pi(q,\omega)=\langle[n,n]\rangle=2N_0\zeta^2\left[\frac{1-f}{\zeta^2-\omega^2}+\frac{\lambda_0f^2}{\lambda_0f\zeta^2-(1+\lambda_0f)(\omega^2-\omega_p^2)}\right] \,, \tag{6}$$

where $\lambda_0=\lambda(\omega_Q/2\Delta)^2$, $f=(2\Delta)^2F$, and ω_p is the CDW pinning frequency, which we have introduced by hand since the new mode below T_c is identified with the LRA sliding mode if $\omega_p=0$. For example, such a modification is justified from the phase Hamiltonian by Fukuyama and Lee.[8] Equation (6) contains two poles; the first pole describes the density fluctuation in the normal conductor while the second pole is the pinned sliding mode.

First let us consider the longitudinal sound velocity. Making use of Eq. (1), we find

$$c=c_0\left[1-2\lambda\left(1-\hat{f}+\frac{\lambda_0\hat{f}^2\zeta^2}{\lambda_0\hat{f}\zeta^2+(1+\lambda_0\hat{f})\omega_p^2}\right)\right]^{1/2} \tag{7}$$

where we made use of the fact that $\omega/\zeta=c/v\ll1$. Here

$$\hat{f}=\lim_{\omega\to0}f\cong\rho_s(T)/\rho \,, \tag{8}$$

and $\rho_s(T)$ is the superfluid density in a BCS superconductor. In the absence of CDW pinning ($\omega_p=0$) Eq. (7) becomes

$$c=c_0(1-2\lambda)^{1/2} \,. \tag{9}$$

The sound velocity is unaffected by the CDW transition. On the other hand, when the CDW is pinned, Eq. (7) yields

$$c=c_0[1-2\lambda(1-\hat{f})]^{1/2} \,, \tag{10}$$

since in most cases $\zeta \ll \omega_p$. The sound velocity c increases upon entrance into the CDW state. Equation (10) may be compared with the temperature dependence[3] of Young's modulus Y in a CDW of TaS_3, which is shown in Fig. 1. Within the present model $Y \propto c^2$, which gives

$$(\Delta Y) Y_n^{-1} \cong \frac{2\lambda}{1-2\lambda} \hat{f} \ , \tag{11}$$

where $\Delta Y = Y - Y_n$ and Y_n is Young's modulus in the normal state. Figure 1 shows that a choice of $2\lambda = 0.062$ gives a fair description of the observed change in Young's modulus, although the experimental result exhibits more curvature in the vicinity of $T = T_c$ whereas the theoretical expression is quite linear in $T_c - T$. Perhaps the inclusion of the thermal fluctuations in Δ eliminates this discrepancy, since the temperature dependence of Y just above $T = T_c$ indicates the presence of such fluctuations.

The present model provides a simple interpretation of the observed field dependence of Young's modulus.[9] When $E > E_T$, the threshold electric field, we may think of the Young's modulus in a partially pinned CDW, when a portion of the CDW starts sliding. Then Eq. (11) is replaced by

$$(\Delta Y) Y_n^{-1} = \frac{2\lambda}{1-2\lambda} \hat{f} P(E) \ , \tag{12}$$

where $P(E)$ is the pinned portion of CDW; $P(E)$ is unity until $E = E_T$. For $E > E_T$, $P(E)$ decreases monotonically from unity and vanishes at another critical field E_c when all parts of the CDW is sliding. However, at the present stage it is difficult to predict the functional form of $P(E)$, since $P(E)$ arises most likely from the spatial inhomogeneity in ω_p.

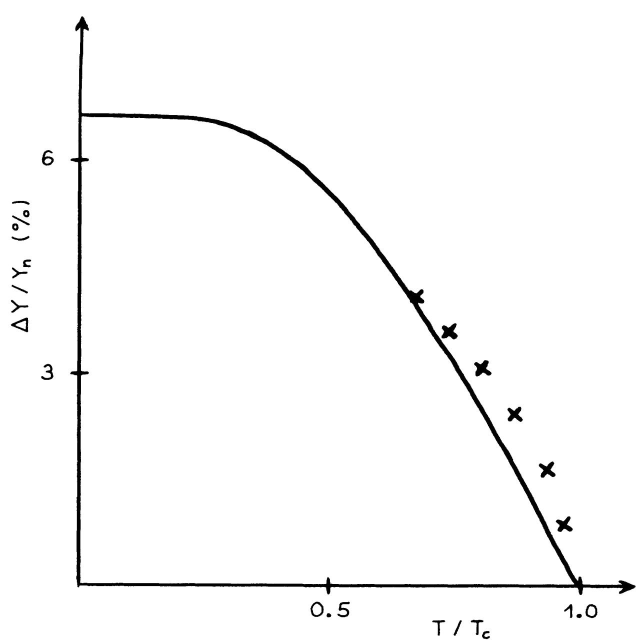

FIG. 1. Temperature dependence of Young's modulus. The crosses are experimental values taken from Ref. 3. The full line corresponds to Eq. (11) with $2\lambda = 0.062$.

To make the theory more concrete, we assume in the following that a CDW splits into domains with individual (or local) threshold fields. Furthermore, the local threshold field is distributed uniformly between E_T and E_c. Then we will have

$$\begin{aligned} P(E) &= 1 \text{ for } E < E_T \\ &= (E_c - E)/(E_c - E_T) \text{ for } E_c > E > E_T \\ &= 0 \text{ for } E > E_c \ . \end{aligned} \tag{13}$$

Substituting $P(E)$ thus constructed into Eq. (12), Eq. (12) describes the main feature of the observed field dependence[2-4] of Young's modulus. $[Y - Y(0)]/Y(0)$ will decrease above E_T and the effect is stronger at lower temperatures. Here $Y(0)$ means Y at zero field. Furthermore, if we assume that the CDW current I_{CDW} associated with a domain with local $E_T(x)$ is proportional[10] to $E - E_T(x)$ when $E > E_T(x)$, we will obtain

$$\begin{aligned} I_{CDW} &= 0 \text{ for } E < E_T \\ &= \tfrac{1}{2} A (E - E_T)^2/(E_c - E_T) \text{ for } E_T < E < E_c \\ &= A[E - \tfrac{1}{2}(E_T + E_c)] \text{ for } E > E_c \ , \end{aligned} \tag{14}$$

where A is a temperature-dependent constant independent of E. Equation (14), together with Eq. (12), gives the observed I_{CDW} dependence of $Y(0) - Y(E)$ (Refs. 2 and 3)

$$Y(0) - Y(E) \propto (I_{CDW})^{1/2} \tag{15}$$

for $E_T < E < E_c$.

In order to describe the field dependence of the dissipation it is necessary to incorporate the quasiparticle damping which is beyond the present analysis.

Second, making use of the charge conservation the frequency-dependent conductivity is obtained from Eq. (6) as

$$\sigma(\omega) = \frac{e^2 N}{m} (i\omega)^{-1} \times \left[f_0 - 1 - f_0 (1 + \lambda_0^{-1} f_0^{-1})^{-1} \frac{\omega^2}{\omega^2 - \omega_p^2} \right] \ , \tag{16}$$

where

$$\begin{aligned} f_0(\omega) &= \lim_{q \to 0} (2\Delta)^2 F \\ &= (2\Delta)^2 \int_\Delta^\infty dE \tanh\left[\frac{\beta}{2} E\right] \\ &\quad \times (E^2 - \Delta^2)^{-1/2} (4E^2 - \omega^2)^{-1} \ . \end{aligned} \tag{17}$$

For $\omega_p = 0$ and $T = 0$, Eq. (16) reduces to the classical result of LRA. Furthermore, Eq. (16) allows us to define m^*/m for $T \neq 0$ as

$$m^*/m = 1 + \lambda_0^{-1} f_0^{-1}(0) \ , \tag{18}$$

which again reduces to the LRA result for $T = 0$ where $f_0^{-1}(0) = 1$. On the other hand, in the vicinity of the transition temperature the phason mass m^* approaches rapidly the electron mass where Eq. (18) is approximately given by

$$m^*/m = 1 + 16 T \Delta(T) / \pi \lambda \omega_Q^2 \ . \tag{19}$$

Both of us wish to thank Peter Fulde for his interest in this work and for his hospitality at the Max-Planck-Institut. One of us (K.M.) gratefully acknowledges the support of the Alexander von Humboldt Foundation. This work is in part supported by the National Science Foundation under Grants No. DMR82-14525 and No. DMR86-11829.

---

*Permanent address: Department of Physics, University of Southern California, Los Angeles, CA 90089-0484.

†Permanent address: Central Research Institute for Physics, H-1525 Budapest 114, P.O. Box 49, Hungary.

[1]See, *Charge-Density Waves in Solids,* edited by G. Hutiray and J. Solyom, Lecture Notes in Physics, Vol. 217 (Springer-Verlag, New York, 1985); *Proceedings of the Yamada Conference on Physics and Chemistry of Quasi-One-Dimensional Conductors* [Physica B **143** (1986)].

[2]J. W. Brill and W. Roark, Phys. Rev. Lett. **53**, 846 (1984).

[3]J. W. Brill, W. Roark, and G. Minton, Phys. Rev. B **33**, 6831 (1986).

[4]G. Mozurkewich, P. M. Chaikin, W. G. Clark, and G. Grüner, in *Change-Density Waves in Solids,* Ref. 1, p. 353.

[5]P. A. Lee, T. M. Rice, and P. W. Anderson, Solid State Commun. **14**, 703 (1974).

[6]See, for example, A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1963), pp. 178–182.

[7]A. Virosztek and K. Maki, Phys. Rev. B **35**, 1954 (1987).

[8]H. Fukuyama and P. A. Lee, Phys. Rev. B **17**, 535 (1978).

[9]For earlier models, see S. N. Coppersmith and C. M. Varma, Phys. Rev. B **30**, 3566 (1984); L. Sneddon, Phys. Rev. Lett. **56**, 1194 (1986). In spirit the second model is very close to ours.

[10]Here we assume that the domain motion is viscous and the driving force is proportional to $E - E_T(x)$.