Dynamics of charge-density waves in the presence of free carriers

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(Received 15 March 1979)

The response of an unpinned, incommensurate charge-density wave (CDW) to external perturbations in the presence of free quasiparticles is studied. The CDW can act as a charged lattice but the proportion of the total charge density assigned to the CDW and to quasiparticles depends on the external conditions. If the collisions between quasiparticles can be ignored, the effective charge of the CDW is different in the static and dynamic limits. In the static limit the quasiparticles relax to screen spatial variations and the form is analogous to that used for superfluids. In the dynamic limit the quasiparticles do not renormalize the effective charge. In the presence of collisions the effective charge depends on the distribution of quasiparticles which in turn depends on the relative importance of various scattering rates. In general, a simple two-fluid model is not applicable.

I. INTRODUCTION

The discovery of charge-density wave states (CDW) in several classes of compounds sparked a new interest in their properties. The earliest theories of CDW were put forward in the 1950's by Peierls[1] and Frohlich[2] for one-dimensional metals. Frohlich[2] recognized that it should be possible to carry a current by drifting the electron fluid relative to the lattice and indeed at the time, prior to BCS, was proposing to explain superconductivity in this way. Subsequent work has shown, however, that the motion of the electron fluid, which must in turn drift the CDW, will be inhibited by the presence of impurities,[3–6] etc., which are located in the background lattice and act to pin the CDW. No dc conductivity linear in the applied field can come from CDW, but nonlinear conductivity is possible.[3,7] Very recently, some striking nonlinear conductivity experiments were made on $NbSe_3$ by Ong and Monceau[8] and led to the suggestion that a depinning of the CDW by an electric field may have been achieved in this material. The theory of such nonlinear conduction from CDW is the subject of a companion paper.[9]

In this paper we will be concerned about the description of a CDW in external fields in the presence of free quasiparticles. Several years ago Lee, Rice, and Anderson[3] showed that the electrical conductivity of a one-dimensional incommensurate Peierls insulator could be described by motion of charge-density wave (CDW) as a whole. The CDW behaved as a charged lattice and carried the full electronic charge but had a large mass. In the presence of free carriers we will show here that a simple two-fluid model with a lattice carrying an effective charge does not work. If the collisions between quasiparticles can be ignored then the discussion can be divided into the static and dynamic limits. In the static limit the quasiparticles relax to screen out spatial variations and the result for the effective charge associated with displacement of the CDW lattice is analogous to that familiar from the theory of superfluids. In the dynamic or high-frequency limit the response of the two systems is less strongly coupled and the effective charge is different. A similar difference is found in the effective mass associated with motion of the CDW. We present both a phenomenological discussion and a microscopic calculation of the response in the collisionless regime. This difference between static and dynamic limits has been overlooked in the microscopic treatment which Schuster[10] gave.

In practice we must include collisions and this leads in general to a form for the effective charge which depends on the distribution of quasiparticles which in turn depends on both the detailed nature of the collision processes and on the type of external perturbation. If a single relaxation time can be used in the Boltzmann equation governing the quasiparticles then the response to a uniform electric field coincides with the dynamic limit in the collisionless regime, a result obtained recently by Boriack and Overhauser.[11] Near to the critical temperature, however, umklapp scattering off the CDW is weak and a different description is appropriate. The discussion we give in this paper only pertains to setting up the coupled equations governing the combined motion of the CDW and quasiparticles. The solution of these coupled equations will, for example, determine the total force on a pinned CDW in an external field or the drift velocity of an unpinned CDW.[9]

The paper is organized as follows. In Sec. II the phenomenological description is given and the response under general conditions is discussed. In Secs. III and IV a microscopic calculation is presented which is in essence a generalized random-phase approximation both for short- and long-range forces,

and which displays the difference between dynamic and static limits. In this latter part collisions are introduced only with the single relaxation-time approximation.

II. PHENOMENOLOGICAL DESCRIPTION

The conductivity in the presence of a CDW consists of two parts. One is a collective part due to motion of the CDW as a whole and the second is the contribution of single particles which arise from the thermal excitation across the gap and possibly from a remnant portion of Fermi surface. The issue which concerns us is the division of the conductivity into collective and single-particle contributions or in other words the proper definition of the effective charge of the CDW.

Throughout this paper we will ignore fluctuations and use a mean-field theory description. For convenience in evaluating integrals over the band structure we will specialize to one-dimensional energy bands but we do not consider the effects of fluctuations which would be essential to describe a truly one-dimensional metal. If the energy bands in the normal state are given by $\epsilon_{\vec{k}}$ then the single-particle spectrum in the presence of the CDW is $\zeta_{\vec{k}} \pm E_{\vec{k}}$ where

$$\zeta_{\vec{k}} = \tfrac{1}{2}(\epsilon_{\vec{k}+\vec{Q}} + \epsilon_{\vec{k}}), \quad E_{\vec{k}}^2 = \xi_{\vec{k}}^2 + \Delta^2 \ , \qquad \xi_{\vec{k}} = \tfrac{1}{2}(\epsilon_{\vec{k}+\vec{Q}} - \epsilon_{\vec{k}}) \ , \tag{2.1}$$

with Δ and $\vec{Q}$ as the CDW energy gap and wave vector. In the Peierls case (i.e., one-dimensional energy bands) $Q = 2k_F$ and $\zeta_{\vec{k}} \equiv 0$, where we measure energies from the Fermi energy.

Consider first if the CDW is unable to move. Then we have a new energy band structure and we can simply calculate the plasma frequency associated with the thermally excited carriers $\omega_{p,n}$ just as one does for any semiconductor.

$$\omega_{p,n}^2 = -4\pi e^2 \sum_{\vec{k}\sigma} \left(\frac{\partial E_{\vec{k}}}{\partial \vec{k}} \right)^2 \frac{\partial f(E_{\vec{k}})}{\partial E_{\vec{k}}} \ , \tag{2.2}$$

$$= -4\pi e^2 V_F^2 \sum_{\vec{k}\sigma} \frac{\xi_{\vec{k}}^2}{E_{\vec{k}}^2} \frac{\partial f(E_{\vec{k}})}{\partial E_{\vec{k}}} \ , \tag{2.3}$$

where f is Fermi function and V_F is the Fermi velocity. If we replace the electron-phonon interaction simply by an attractive electron-electron potential of appropriate strength, then the Hamiltonian would commute with the total electron momentum. The total oscillator strength, which is determined by $\omega_p^2 = 4\pi e^2 \bar{\rho}/m$ where $\bar{\rho}$ is the electron density and $m (= k_F V_F^{-1})$ is the mass, can then be partitioned into the part due to the thermally excited carriers $\omega_{p,n}^2$ and the remainder

$$\omega_{p,c}^2 = \omega_p^2 - \omega_{p,n}^2 \tag{2.4}$$

is to be associated with the condensate. The fractional-charge density ρ_c is associated with the condensate. An effective charge ρ_c can then be defined by $\omega_{p,c}^2 = 4\pi e^2 \rho_c \bar{\rho}/m$.

There are also retardation effects associated with the electron-phonon interaction, in addition to the effective electron-electron attraction, and these lead to a large mass enhancement (m_L/m) for the collective contribution. The spectral weight taken out by this mass enhancement due to retardation appears in the single-particle transitions across the Peierls gap.[3] The low-frequency $(\omega << \Delta)$ dielectric function $\epsilon(\omega)$ can then be written

$$\epsilon(\omega) = 1 + \alpha_{\text{ib}} - \frac{\omega_{p,n}^2}{\omega^2} - \frac{\omega_{p,c}^2}{\omega^2} \frac{m}{m_L} \ , \tag{2.5}$$

where α_{ib} is the interband polarizability.

A second approach to determine the effective charge of the CDW is to use the relationship between the charge density and the gradient of the phase ϕ of the CDW. This can be calculated from static considerations alone. Consider a very long-wavelength oscillation of the phase in a Peierls insulator. Then the chemical potential will be constant but locally the period will change from $2k_F$ to $2k_F + \nabla\phi$. Such a change in period leads to a change in the local density. The energy spectrum (for $k > 0$) is changed to

$$E'(k) = \pm E(k - q) + V_F q \ , \tag{2.6}$$

where $q = \frac{1}{2}\nabla\phi$. The change in density is

$$\delta\rho = 2 \sum_{k>0,\sigma} [f(-E(k-q) + V_F q) - f(-E_k) + f(E(k-q) + V_F q) - f(E_k)] \ , \tag{2.7}$$

where the factor of 2 comes from summing over $k < 0$ and $k > 0$. Rewriting Eq. (2.7) as

$$\delta\rho = \frac{2q}{\pi} + 2 \sum_{k,\sigma} [f(E(k-q) + V_F q) - f(E(k-q) - V_F q)] \ , \tag{2.8}$$

transforming to a new variable $k' = k - q$, and neglecting end effects we expand to obtain

$$\delta\rho = \frac{2q}{\pi} + 4 V_F q \sum_{k,\sigma} \frac{\partial f(E_k)}{\partial E_k} \ . \tag{2.9}$$

This can be written

$$\frac{\delta\rho}{\bar{\rho}} = \frac{\nabla\phi}{2k_F} \tilde{\rho}_c \ , \tag{2.10}$$

where $\tilde{\rho}_c$ is interpreted as the fractional-charge density that is associated with a static distortion of the

condensate and

$$\tilde{\rho}_c = 1 + \frac{\pi k_F}{m} \sum_{k,\sigma} \frac{\partial f(E_k)}{\partial E_k} \quad . \tag{2.11}$$

We note that except at $T=0$, $\tilde{\rho}_c$ and ρ_c defined from Eq. (2.4) are different. This is seen most easily as $T \to T_c$ or $\Delta \to 0$, when $\rho_c \sim \Delta$ but $\tilde{\rho}_c \sim \Delta^2$. This leads immediately to the question of the proper definition of effective charge relating the collective contribution to the current J_c to the time derivative of the phase[4]

$$J_c = e\bar{\rho}\rho_c' \dot{\phi}/2k_F \quad . \tag{2.12}$$

To be consistent with Eq. (2.4) we should have $\rho_c' = \rho_c$. On the other hand it is tempting to use an equation of continuity together with Eq. (2.10) which will lead to $\rho_c' = \tilde{\rho}_c$. The origin of this problem is simply the nonanalytic response of the Fermi liquid of thermally excited quasiparticles in the collisionless regime. Equation (2.12) must be interpreted as the dynamic limit and $\rho_c' = \rho_c$ is the correct answer.

In practice we must include the effects of collisions. This introduces the further complication that the proportionality constant ρ_n' between $\vec{J}_n$, the current contributed by the excited particles, and $\vec{K}$, their total crystal momentum, depends on the shape of their distribution, which in general depends on both the detailed nature of the collision processes and on the type of external perturbation. It remains true, however, that if a translationally invariant background is assumed, then $\rho_n' + \rho_c' = 1$. The result ρ_c found above may be easily derived if the distribution is assumed determined solely by the driving field

$$\delta f_k = \frac{\partial f}{\partial k}\frac{E}{i\omega} = \frac{\partial f}{\partial k} K \quad .$$

Then $J_n = \rho_n' K$ with $\rho_n' = 1 - \rho_c$. The expression for the plasma frequency then follows from simple arguments. The same result for ρ_n' applies even when collisions are important, providing the simple ansatz for the shape of the distribution $\delta f_k = (\partial f/\partial k)K$ is again used. This is the standard single relaxation-time approximation for the Boltzmann equation. This may not be correct in general, especially for perturbations other than an electric field, a situation which may arise when the CDW and the quasiparticle are drifting at different velocities. The point is that the thermally excited particles do not in general form a second independent fluid that can rigorously be treated in terms of a few macroscopic variables (a hydrodynamic treatment), but should strictly be treated individually (i.e., by a Boltzmann equation) for each situation.

In Ref. 9 we have written down a phenomenological description of the coupled drift of the CDW and quasiparticles in the presence of an electric field based on the simple ansatz. This should be viewed at best as a variational solution to the Boltzmann equation. We should point out that there is at least one particular situation where the excitations may be properly treated as a second fluid and a different distribution is more appropriate. Suppose that above T_c forward scattering is dominant (for example, scattering by long-wavelength thermal phonons at low temperatures). Then just below T_c collisions that conserve the crystal momentum of the excited particles will be much more rapid than those that do not — umklapp scattering off the charge-density wave obviously disappears above T_c, and so must become slow (rate $\propto \Delta^2$) near T_c. Under these conditions the excitations relax rapidly under crystal-momentum–conserving collisions to an equilibrium with an average velocity $\vec{v}$ (that may be different from the charge-density wave velocity) with the distribution

$$\delta f_k \propto -\frac{\partial f}{\partial E}\vec{k}\cdot\vec{v} \quad . \tag{2.13}$$

This is the usual expression for a two-fluid model and follows from setting the crystal-momentum–conserving part of the collision integral to zero and not from any assumptions of Galilean invariance. With the distribution Eq. (2.13) J and K are related by yet another effective charge. This treatment of the region near T_c is very reminiscent of the discussion by Pethick and Smith[12] of the corresponding region in a superconductor where again it is profitable to introduce an additional slowly relaxing (quasihydrodynamic) variable — in their case the "superfluid charge." The particular collision process that becomes slow is, however, quite different in the two cases.

Allender, Bray, and Bardeen[13] arrived at a form for the effective charge at $T \sim T_c$ which is equivalent to $\tilde{\rho}_c$ in that limit. They worked in the laboratory frame with a time-dependent potential and evaluated the free energy by summing over the eigenvalue spectrum $\lambda'(\vec{D})$ $[\equiv E(\vec{k} - m\vec{D}) + \vec{D}\cdot\vec{k}]$ in the presence of a CDW drifting with a velocity $\vec{D}$ and then expanded the free energy to order D^2 to obtain $\tilde{\rho}_c$. Collisions were not explicitly included. The problem is that, as pointed out by Boriack and Overhauser,[14] the energy defined by the mean value of $i\partial/\partial t$ is not λ' but $E(\vec{k} - m\vec{D}) + m\vec{D}\cdot\partial E/\partial\vec{k}$. Using this value one can recover the answer ρ_c in agreement with our result in the collisionless regime. This is also in agreement with Boriack and Overhauser[11] if one interprets their parameter γ appropriately and takes a one-dimensional band structure.

III. PHASE MODE WITH SHORT-RANGE FORCES ONLY

We begin our discussion of microscopic theory by considering the dispersion of the phase mode. For the present we will restrict our attention to a system with only short-range forces. We will study the influ-

ence of the free carriers on the dispersion of the phase mode. To make the model a little more realistic we will include also a pinning potential which we take as a weak external potential whose period is commensurate with that of the CDW.

The Hamiltonian in the standard Frohlich form is

$$H_0=\sum_{\vec{k}\sigma}\epsilon_{\vec{k}}c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma}+\sum_{\vec{q}}\omega_{\vec{q}}\left(b^{\dagger}_{\vec{q}}b_{\vec{q}}+b^{\dagger}_{-\vec{q}}b_{-\vec{q}}\right)+\sum_{\vec{q}}\left(\frac{ig}{(N)^{1/2}}\sum_{\vec{k}\sigma}c^{\dagger}_{\vec{k}+\vec{q}\sigma}c_{\vec{k}\sigma}(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})+\text{c.c.}\right), \tag{3.1}$$

where $c^{\dagger}_{\vec{k}}$ and $b^{\dagger}_{\vec{k}}$ are electron and phonon creation operators, ω_q is the phonon energy, and g is electron-phonon coupling constant. The presence of an external potential with wave vector $\vec{Q}$ adds a term

$$H_{\text{imp}}=\sum_{\vec{k}\sigma}V_{\vec{Q}}c^{\dagger}_{\vec{k}+\vec{Q}\sigma}c_{\vec{k}\sigma}+V^{*}_{\vec{Q}}c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}+\vec{Q}\sigma}\ . \tag{3.2}$$

In mean-field theory, a single-phonon mode is taken to be macroscopically occupied in the presence of the CDW. Denoting this occupation number by

$$w=\langle b_{\vec{Q}}+b^{\dagger}_{-\vec{Q}}\rangle/(N)^{1/2} \tag{3.3}$$

leads to an effective potential seen by the electrons of $igw+V_Q$. After diagonalizing the Hamiltonian and minimizing the free energy with respect to the choice of w, one obtains the pair of gap equations

$$\omega_Q w^{*}=\sum_{\vec{k},\sigma}\frac{igV^{*}_{Q}+g^2w^{*}}{E_{\vec{k}}}\left[f(\zeta_{\vec{k}}-E_{\vec{k}})-f(\zeta_{\vec{k}}+E_{\vec{k}})\right], \tag{3.4}$$

$$\omega_Q w=\sum_{\vec{k},\sigma}\frac{-igV_{Q}+g^2w}{E_{\vec{k}}}\left[f(\zeta_{\vec{k}}-E_{\vec{k}})-f(\zeta_{\vec{k}}+E_{\vec{k}})\right], \tag{3.5}$$

where the energy gap $\Delta=V_Q+igw$. Multiplying Eq. (3.4) by w and Eq. (3.5) by w^* and subtracting leads to

$$V^{*}_{Q}w=-V_Qw^{*}\ , \tag{3.6}$$

or if we let $w=|w|\exp(i\phi)$ and $V_Q=|V_Q|\exp(i\chi)$, then Eq. (3.6) is satisfied if $\phi=\chi\pm\frac{1}{2}\pi$. The (+) sign leads to a maximum in the free energy and the (−) to a minimum. The presence of the external potential pins the phase of the lattice distortion.

The pinning shows up directly if we look at the phason collective mode. Denoting the phonon propagators by

$$D_{m,n}(\vec{q},t)=-\frac{i}{\omega_Q}\langle T[b_{m\vec{Q}+\vec{q}}(t)b^{\dagger}_{n\vec{Q}+\vec{q}}(0)]\rangle \tag{3.7}$$

with $m,n=\pm$ and the electronic propagators

$$G_{m,n}(\vec{k},t)=i\langle T[c_{\vec{k}+m\vec{Q}/2}(t)c^{\dagger}_{\vec{k}+n\vec{Q}/2}(0)]\rangle\ , \tag{3.8}$$

then the thermal Green's function can be written in matrix form using the Matsubara notation $\omega_n=(2n+1)\pi T$,

$$G^{-1}(\vec{k},\omega_n)=\begin{pmatrix} i\omega_n-\epsilon_{\vec{k}+\vec{Q}/2} & -\Delta \\ -\Delta^{*} & i\omega_n-\epsilon_{\vec{k}-\vec{Q}/2}\end{pmatrix}. \tag{3.9}$$

The phase mode shows up as a low-frequency mode by considering the Dyson equation for the combination[3]

$$D_{++}(\vec{q},\omega_n)-D_{\pm}(\vec{q},\omega_n)=D_0\left[1+g^2\omega_QD_0T\sum_{\vec{k},\nu_m,\sigma}\text{Tr}[(i\tau_2)G(\vec{k},\nu_m)(-i\tau_2)G(\vec{k}+\vec{q},\omega_n+\nu_m)]\right]^{-1}, \tag{3.10}$$

where τ_2 is one of the Pauli matrices

$$\tau_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \tag{3.11}$$

and $D_0^{-1}=\omega_n^2+\omega_Q^2$.

The frequency of the pinned phase mode ω_g is given by the zeros of the denominator in Eq. (3.10) after it is analytically continued to the real axis. In the long-wavelength limit ($q\to 0$) we obtain

$$0=-\omega_g^2+\omega_Q^2+2g^2\omega_Q\sum_{\vec{k},\sigma}\frac{2E_{\vec{k}}r_{\vec{k}}}{\omega_g^2-4E^2_{\vec{k}}}\ , \tag{3.12}$$

with

$$r_{\vec{k}}=1-f(-\zeta_{\vec{k}}+E_{\vec{k}})-f(\zeta_{\vec{k}}+E_{\vec{k}})\ .$$

Since we are only interested in the low-frequency limit $\omega<<|\Delta|$ we can expand the last term in Eq. (3.12) to give

$$\omega_g^2\left(1+g^2\omega_Q\sum_{\vec{k}\sigma}r_{\vec{k}}/4E^3_{\vec{k}}\right)=\omega_Q^2-g^2\omega_Q\sum_{\vec{k}\sigma}r_{\vec{k}}/E_{\vec{k}}\ . \tag{3.13}$$

Now the right-hand side of Eq. (3.13) can be rewritten with the help of the gap Eq. (3.4), leading to the

result

$$\omega_g^2=\omega_Q g\left|\frac{V_Q}{w}\right|\left|\sum_{\vec{k}\sigma} r_{\vec{k}} E_{\vec{k}}^{-1}\right|\left(1+g^2\omega_Q\sum_{\vec{k}\sigma} r_{\vec{k}}/4E_{\vec{k}}^3\right)^{-1} . \tag{3.14}$$

Using the gap Eq. (3.4) and linearizing in V_Q we obtain

$$\omega_g^2=\left(\frac{m}{m_L}\right)\left|\frac{V_Q}{\Delta}\right|\left|\frac{\omega_Q}{g^2}\right|\left(\sum_{k\sigma} r_{\vec{k}}/4E_{\vec{k}}^3\right)^{-1} , \tag{3.15}$$

with

$$\frac{m_L}{m}=1+\left(g^2\omega_Q\sum_{\vec{k}\sigma} r_k/4E_k^3\right)^{-1} . \tag{3.16}$$

Examining the result first for a one-dimensional Peierls insulator at zero temperature, the integrals can be carried out at once to give

$$\omega_g^2=4|\Delta V_Q|\lambda^{-1}/(1+4\Delta^2/\lambda\omega_Q^2) , \tag{3.17}$$

where λ is the dimensionless electron-phonon coupling constant $\lambda=2g^2N(0)/\omega_Q$ and $N(0)=2/\pi V_F$ is the density of states at the Fermi level. The term in the parentheses is the well-known effective mass m_L/m of the CDW first derived by Fröhlich[2] due to slow response time of the phonons. The numerator in Eq. (3.17) can be derived simply by writing down the kinetic energy density of a moving CDW and the potential energy density in the pinning potential

$$E(\phi)=\tfrac{1}{2}nm_L\left(\frac{d(\phi/Q)}{dt}\right)^2-2|V_Q|\rho_1\cos\phi , \tag{3.18}$$

where ρ_1 $[=2N(0)\Delta/\lambda]$ is the amplitude of the CDW. Solving for frequency of the pinning mode gives

$$\omega_g^2=2N(0)|V_Q\Delta|\lambda^{-1}/\tfrac{1}{2}nm_L Q^{-2} , \tag{3.19}$$

which can be readily brought into agreement with Eq. (3.17). The frequency of the pinned phase mode is determined simply by balancing the kinetic energy of CDW motion against the pinning potential.

The derivation of Eq. (3.15) is quite general and can be used in cases where there are free carriers either from a remnant Fermi surface or quasiparticle excitations in a Peierls insulator at finite temperature. In this case we must consider the Greens function product in Eq. (3.10) which has both interband terms involving transitions across the Peierls gap and intraband terms. In the limit $q\to 0$ and ω finite which we have considered only the interband terms contribute as in Eq. (3.12). The intraband terms however depend critically on the order in which the limits $q\to 0$ and $\omega\to 0$ are taken as is well known for products of fermion propagators. At finite q, then we must consider the intraband terms.

First we consider the evaluation of Eq. (3.10) for general (q,ω) but with $V_F q << \Delta$ and $\omega << \Delta$. Then Eq. (3.12) becomes (setting $\zeta_k\equiv 0$ for simplicity)

$$0=-\omega_g^2(\vec{q})+\omega_Q^2+2g^2\omega_Q \times\sum_{\vec{k},\sigma}\left(\frac{2E_{\vec{k}}r_{\vec{k}}}{\omega_g^2(\vec{q})-4E_{\vec{k}}^2}-\frac{2(E_{\vec{k}+q}-E_{\vec{k}})^2p_{k,q}^2\,\partial f/\partial E_{\vec{k}}}{\omega_g^2(\vec{q})-(E_{\vec{k}+\vec{q}}-E_{\vec{k}})^2}\right) , \tag{3.20}$$

where the matrix element $p_{k,q}^2\to V_F^2q^2\Delta^2/4E_k^4$ as $q\to 0$. The behavior of the intraband part (the last term) depends on the average value of the $\vec{q}\cdot\vec{v}_k/\omega$, with $\vec{v}_k=\partial E_{\vec{k}}/\partial\vec{k}$. Because the dispersion of the phase mode is characterized by a large mass $\sim(mm_L)^{1/2}$ it will rapidly pass into the regime where $\vec{q}\cdot\vec{v}>>\omega_g(q)$. It is the static response that controls the dispersion relation in this regime. The general behavior of the dispersion relation is quite complicated. If we pass to the limit $\omega_g(q)>>\omega_g(0)$, or equivalently ignore the external field, one obtains

$$\omega_g^2(q)=\frac{m}{m_1}V_F^2q^2 , \tag{3.21}$$

where the mass ratio m/m_1 can be expressed most conveniently as a Matsubara sum

$$\frac{m_1}{m_1}=1+\left(g^2\omega_Q T\sum_{k,n}\frac{1}{(\omega_n^2+\xi_k^2+\Delta^2)^2}\right)^{-1} . \tag{3.22}$$

At $T=0$ K in a one-dimensional Peierls insulator the two masses m_L and m_1 are the same. However at finite temperature they differ significantly. As $T\to T_c$ and $\Delta\to 0$ one finds from Eq. (3.16) that $m_L/m-1\sim T_c\Delta/\lambda\omega_Q^2\to 0$ while $m_1/m\sim T_c^2/\lambda\omega_Q^2$ continues to be large. This difference in the effective masses reflects the behavior in the dynamic and the static limits. We will return to this point in Sec. IV when we discuss the effective charge.

The above description applies in the collisionless regime. Collisions affect primarily the intraband term and if one makes the simplest approximation using a single relaxation time then the collisionless form is modified by making the replacement $\omega_g^2\to\omega_g^2-i\omega_g\tau^{-1}$ where τ is the relaxation time. In this simple limit all distinction between umklapp and nonumklapp collisions is lost. As we discussed in Sec. II the relative weight of these two processes is important in determining the distribution functions and hence the effective charge. The microscopic treatment given above is based on a random-phase approximation and this treatment would require substantial modification to go beyond the single relaxation-time approximation.

IV. ELECTROMAGNETIC PROPERTIES

The response to an external electric field is described by the dielectric function which is expressed as the sum of the proper polarizabilities. In addition to the contributions from interband transitions and from the free carriers there is the possibility of motion of the CDW as a whole in the electric field as we discussed in Sec. II. In a microscopic calculation this appears as a coupling to the phase mode and the magnitude of this coupling will determine the effective charge of the CDW.

The polarizability of the phase mode can be written

$$\alpha_p(\vec{q},\omega) = -\frac{|M(\vec{q},\omega)|^2}{\omega^2 + \pi(\vec{q},\omega)} \quad . \tag{4.1}$$

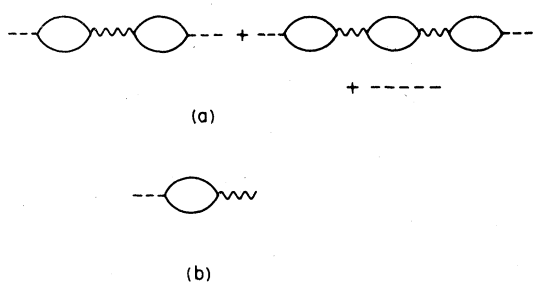

FIG. 1. (a) Diagrammatic representation of the conductivity due to the collective mode. (b) The matrix element M.

The matrix element M is given by the diagram (b) in Fig. 1 as

$$M(\vec{q},i\nu) = (4\pi\omega_0)^{1/2}\frac{ge}{q}T\sum_{\vec{k},\sigma,n}\mathrm{Tr}[1G(\vec{k}+\vec{q},i\omega_n+i\nu)(i\tau_2)G(\vec{k},i\omega_n)] \quad . \tag{4.2}$$

After making the analytic continuation to the real axis and taking the $(V_F q,\omega) << \Delta$ limit, we find two terms again

$$M(q,\omega) = \frac{(4\pi\omega_Q)^{1/2}eg}{q}\Delta\sum_{\vec{k},\sigma}\vec{v}_F\cdot\vec{q}\left[\frac{1}{E_{\vec{k}}^3}\tanh(\tfrac{1}{2}\beta E_{\vec{k}}) + \frac{(\partial E_{\vec{k}}/\partial\vec{k}\cdot\vec{q})^2 E_{\vec{k}}^{-2}}{\omega^2-(\partial E_{\vec{k}}/\partial\vec{k}\cdot\vec{q})^2}\frac{\partial}{\partial E}[\tanh(\tfrac{1}{2}\beta E)]\right] \quad , \tag{4.3}$$

(where we have set $\zeta_{\vec{k}}\equiv 0$ for simplicity).

The matrix element M describes the coupling of the ionic displacements with the long-wavelength electronic density. It vanishes identically for certain systems. For example, in the case of the SDW in Cr metal, the states coupled belong to two different subbands and the sum of $\vec{k}$ is over a closed piece of Fermi surface.[15] As a result, the sum vanishes identically. The order parameter involves in this case a spatially modulated occupation of d orbitals as well as spin states. By contrast in KCP $[K_2Pt(CN)_4Br_{0.3}\cdot 2H_2O]$, states in the same band are coupled across the Fermi surface and a true CDW results, i.e., the occupation of one orbital is modulated in space. In this case the sum over $\vec{k}$ is restricted to a half space, $\vec{k}\cdot\vec{Q}<0$, and $(\partial\xi/\partial\vec{k})\cdot\vec{q}$ has a fixed value $\approx V_F q$. In the case of tetrathiafulvalenium-tetracyano-p-quinodimethanide (TTF-TCNQ), there are separate electron and hole bands and they make cancelling contributions to M because of their opposite charge. In this case there is a simple physical picture why the CDW does not couple to a uniform electric field. The electron and hole CDW wish to move opposite in the electric field and so the interchain coupling opposes the motion and they are simply polarized. The electric field does not couple to the phase mode which moves the electron and hole CDW together.

Lastly we consider the layered compounds.[16] Again the states that are coupled by the CDW belong to the same band and $M\neq 0$. The CDW in these materials should couple to an electric field, though in the $2H$ polytypes, the topology of the Fermi surface is such that considerable cancellation occurs in the sum and M will be reduced. In the $1T$ polytypes of TaS_2 and $TaSe_2$, the Fermi surface consists of a set of ellipsoidal electron bands and the CDW couples states across the ellipsoids which should give a large value to the matrix element, M.

Turning to the evaluation of M, the second term in Eq. (4.3) depends on the way in which the long-wavelength limit is taken. If ω is held finite while $q\to 0$ the second term in Eq. (4.3) vanishes. Using the results of Sec. III, after some algebra we obtain

$$\alpha_p(0,\omega) = \frac{4\pi e^2}{m_L/m(\omega_g^2-\omega^2)}\sum_{k,\sigma}\frac{V_F^2\Delta^2}{E_k^3}[1-2f(E_k)] \quad . \tag{4.4}$$

This term arises from the change in the occupied wave functions when the ions are displaced. It was derived recently by Boriack and Overhauser.[11] If we use the identity $\Delta^2/E_k^3 \equiv E_k^{-1} - \xi_k^2/E_k^3$ and the gap equation one can show that Eq. (4.4) is identical to the last term on the right-hand side of Eq. (2.5) in the absence of the pinning potential. The microscopic calculation agrees with the phenomenological form and the effective charge agrees with the dynamic value obtained in Sec. III.

The remaining terms in the polarizability from interband transitions across the one electron gap, α_{ib}, and from free carriers, α_f, are contained in Fig. 1(a).

We get

$$\alpha_{ib}(\vec{q},i\nu)+\alpha_f(\vec{q},i\nu)=\frac{4\pi e^2}{q^2}T\sum_{\vec{k},\omega_n,\sigma}\mathrm{Tr}[1G(\vec{k}+\vec{q},\omega_n+\nu)1G(\vec{k},\omega_n)] \tag{4.5}$$

and after making the analytic continuation to the real axis one finds

$$\alpha_{ib}(\vec{q},\omega)+\alpha_c(\vec{q},\omega)=-\frac{4\pi e^2}{q^2}\sum_{\vec{k}\sigma}\frac{(\vec{V}_\xi\cdot\vec{q})^2\Delta^2}{4E_{\vec{k}}^4}\frac{2E_{\vec{k}}}{\omega^2-4E_{\vec{k}}^2}[1-f(\zeta_{\vec{k}}+E_{\vec{k}})-f(-\zeta_{\vec{k}}+E_{\vec{k}})]$$
$$-\frac{4\pi e^2}{q^2}\sum_{\vec{k}\sigma}\frac{(E_{\vec{k}+\vec{q}}\pm\zeta_{\vec{k}+\vec{q}})-(E_{\vec{k}}\pm\zeta_{\vec{k}})}{\omega^2-[(E_{\vec{k}+\vec{q}}\pm\zeta_{\vec{k}+\vec{q}})-(E_{\vec{k}}\pm\zeta_{\vec{k}})]^2}[f(E_{\vec{k}+\vec{q}}\pm\zeta_{\vec{k}+\vec{q}})-f(E_{\vec{k}}\pm\zeta_{\vec{k}})]\ , \tag{4.6}$$

where $\vec{V}_\xi=d\xi_{\vec{k}}/d\vec{k}$ (for one-dimensional bands $V_\xi=V_F$ as we remarked earlier).

It is straightforward to evaluate these expressions and obtain answers in agreement with Eq. (2.5).

In the opposite limit when $\omega\to 0$ first and q remains finite the second term in Eq. (4.3) is nonzero and can cancel part of the first term. In particular as $T\to T_c$, then the first and second term are both finite but cancel exactly so that the total varies as Δ. This can be seen simply by rewriting $M(q,0)$ as a Matsubara sum

$$M(q,0)=(4\pi\omega_Q)^{1/2}\frac{eg}{q}T\times\sum_{k,n,\sigma}\frac{2(\vec{V}_\xi\cdot\vec{q})\Delta}{[(i\omega_n-\zeta_k)^2-\xi_k^2-\Delta^2]^2}\ . \tag{4.7}$$

Clearly $M(q,0)$ vanishes linearly in Δ as $\Delta\to 0$ and $T\to T_c$. The static form of the propagator in the denominator of Eq. (4.1) also is characterized by the static form of the effective mass m_1/m. The criterion which distinguishes the static and dynamic limits in the collisionless regime is $\omega/|\vec{V}_\xi\cdot\vec{q}|<<1$ or $>>1$. In the limit $\omega<<|V_\xi q|$ but $\omega>>\vec{V}_\xi\cdot\vec{q}(m/m_L)^{1/2}$, the static limit of M must be used leading to a different expression for α (with $V_Q\equiv 0$)

$$\alpha_p(\omega<<|\vec{V}_\xi\cdot\vec{q}|)$$
$$=-\frac{4\pi e^2\Delta^2 T}{m_1\omega^2/m}\sum_{\vec{k},n,\sigma}(\vec{V}_\xi\cdot\vec{n})^2[(i\omega_n-\zeta_{\vec{k}})^2-\xi_{\vec{k}}^2-\Delta^2]^{-2} \tag{4.8}$$

In this limit it is the static mass which enters. The spectral weight of the phase mode varies as Δ^2 in the limit $\Delta\to 0$. If we use the spectral weight to identify an effective charge then after a little algebra, one can show that the effective charge in Eq. (4.8) is the static value $\tilde{\rho}_c$ given by Eq. (2.11). We have shown how the two different effective charges of the CDW arise in the microscopic theory and the relaxation of the free carriers is responsible for the different values in the static and dynamic limits.

Again we can simply incorporate collisions within the single relaxation-time assumption by adding a term $i\omega/\tau$ to the denominator of all intraband terms.[17] This modifies the criterion which separates the static and dynamic limit. In particular to achieve the static or space-charge limit it is not sufficient to have $\omega<<|\vec{V}_\xi\cdot\vec{q}|$ but also $\omega\tau^{-1}<<(\vec{V}_\xi\cdot\vec{q})^2$. Under these conditions, the results quoted above for the static limit continue to hold.

V. CONCLUSIONS

CDW in many systems act as a charged lattice. However, they cannot simply be viewed as a rigid lattice of charges because of the presence of free carriers. The free carriers act to screen out any space charge developed by a nonuniform field and in the process renormalize the effective charge that we associate with the CDW. It is important to distinguish the static and dynamic limits carefully — a point overlooked by Schuster.[10] In the static limit the expression for the effective charge resembles that expected by analogy with the theory of superfluids and the spatial variations are screened out by the quasiparticles. But in the dynamic limit the inertial response of the CDW and the quasiparticles are uncoupled. This continues to hold if the collision processes can be characterized by a single relaxation rate as was found also by Boriack and Overhauser. In this case it is the dynamic effective charge ρ_c which determines both the force on the CDW and the current carried by the CDW in an electric field. If the scattering processes are more complicated with, for example, different rates for normal processes and umklapp processes off the CDW, then a two-fluid description will not be valid. The Boltzmann equation governing the quasiparticle distribution must be solved and the response functions evaluated. If the umklapp processes are very weak then crystal momentum is conserved again and a different two-fluid description can be given.

ACKNOWLEDGMENT

The authors are grateful to Professor J. Bardeen for a useful correspondence and for bringing the work of C. Pethick and H. Smith, Ref. 13, to their attention.

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