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Dynamics of the charge-density wave. I. Impurity pinning in a single chain

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We study the effect of impurities on the dynamics of charge-density waves. At low temperature it is a good approximation to restrict our attention to phase fluctuation only. The competition between the random impurity potential and the elastic energy for phase fluctuations leads us naturally to consider two limiting cases. In the strong pinning case the phase is pinned to each impurity site. The pinning frequency and the frequency-dependent conductivity can be calculated. In the weak pinning case the pinning mechanism is more subtle. We show that the system is pinned by effectively breaking up into domains. The domain size is estimated which in turn determines the pinning frequency. The frequency-dependent conductivity and the static dielectric constant are calculated.

I. INTRODUCTION

In the past few years there has been intense interest in the study of charge-density-wave (CDW) formation in one-dimensional conductors.[1-3] Particular attention has been focused on the current-carrying properties of the CDW state.[4-7] The CDW is described by a modulation of the charge density

$$\rho(x) = \bar{\rho} + \rho_0 \cos(Qx + \phi), \tag{1.1}$$

where $\bar{\rho}$ is the uniform density, ρ_0 is the amplitude of the CDW and $Q = 2k_F$ is the wave vector. The phase ϕ describes the location of the CDW relative to the lattice. It was first pointed out by Frohlich[8] that if the wave vector Q is incommensurate with the lattice vector the energy of the CDW state is independent of its location relative to the lattice, i.e., independent of ϕ. In that case the CDW structure can slide through the lattice without resistance. Furthermore in cases where the CDW is formed out of a single band, the CDW structure has a net charge and such a sliding CDW will be current carrying. It has been proposed that fluctuations into the CDW state can account for the conductivity peak observed in the organic conductor tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ). Although the understanding about the conductivity peak is not yet fully definite,[5,6] the situation at low temperatures is slightly less controversial. Lee, Rice, and Anderson[9] have constructed a microscopic mean-field theory for zero temperature and confirmed the current-carrying nature of the CDW state. However, they find that impurity scattering has a profound effect on the behavior of the CDW. More specifically they found that the usual self-energy calculation for the phase motion of the CDW leads to divergence at $\omega = 0$. The reason for this is that the phase variable couples linearly to the impurity potential. This is to be contrasted with the more familiar deformation-potential coupling which is proportional to the gradient of the phase. Lee, Rice, and Anderson concluded that because the coupling is so strong, the CDW is pinned by the impurity potential. Instead of contributing to dc conductivity, the CDW is responsible for a low-frequency peak in the frequency-dependent conductivity. At the same time the low-lying excitations contribute to a large static dielectric constant. A low-lying excitation that can be interpreted as the pinned phase mode has in fact been found in KCP $[K_2Pt(CN)_4BR_{0.3}3 \cdot 2H_2O]$,[10] and all the one-dimensional conductors are known to have dielectric constants of the order of several thousand in the low-temperature insulating phase.[11] It is therefore desirable that a calculation of the frequency-dependent conductivity for a CDW in the presence of impurities be performed. Such a calculation has recently been done by Fukuyama[12] who considered the case of weak impurity scattering. The main approximation made in that work is that for weak impurity scattering the phase deviation is small and can be linearized. However, it has been pointed out recently by Sham and Patton[13] and by Imry and Ma[14] that even for weak impurity scattering, long-range order is impossible in less than four dimensions. A recent generalization[15] to include long-range Coulomb effects reduces this dimensionality from 4 to 3. The important point remains that in less than three dimensions the phase fluctuation can be arbitrarily large. Therefore linearization in the phase variable is not valid for low-frequency excitations and one should instead linearize about some equilibrium phase $\phi_0(x)$. This is the approach we have taken in this paper. We have been able to treat both the weak- and strong-impurity-scattering limit and identify the criterion separating the two extremes. We succeeded in removing certain undesirable features of the previous work. Furthermore our present approach clarifies certain controversies in the literature. In particular Sokol-

off[16] has claimed that weak impurities do not pin the CDW. Our results show that even in the weak-impurity-scattering limit the CDW is pinned at least as far as the linear conductivity is concerned.

II. DYNAMICS OF THE CHARGE-DENSITY WAVE

We consider the dynamics of CDW at low temperature when amplitude fluctuations are negligible. The only dynamical variable we consider is the phase $\phi(x)$. As shown by Fukuyama[12] its dynamics can be described by the effective Hamiltonian

$$H_0 = \pi v' \int dx \left[p^2 + \frac{1}{4\pi^2} \left(\frac{v}{v'} \right)^2 (\nabla\phi)^2 \right], \tag{2.1}$$

where p is the momentum conjugate to ϕ and

$$v = (m/m^*)^{1/2} v_F, \tag{2.2}$$

is the velocity of the phase mode, m^* is the effective mass which can be calculated microscopically,[9] and we have introduced

$$v' = v^2/v_F. \tag{2.3}$$

We refer the reader to Ref. 12 for a derivation of Eq. (2.1) but simply note here that $1/2\pi v'$ plays the role of a mass density and the constants in Eq. (2.1) have been chosen to reproduce the phase mode velocity v.

Next we consider the interaction of the CDW with impurity potential $v(x - R_i)$ located at R_i,

$$H' = \sum_i \int dx\, \rho(x) v(x - R_i). \tag{2.4}$$

We shall assume a short range potential $v(x) = V_0 \delta(x)$, in which case Eq. (2.4) becomes

$$H' = V_0 \rho_0 \sum_i \cos[QR_i + \phi(R_i)]. \tag{2.5}$$

Equations (2.1) and (2.5) are our total Hamiltonian.

We see at once that we are facing a highly nonlinear problem. Furthermore in general $\phi(R_i)$ will not be small. As mentioned in the Introduction, the way we proceed is to find an equilibrium distribution $\phi_0(x)$ for a given impurity distribution and then do a small expansion about it. Before we proceed let us discuss the physical behavior of $\phi_0(x)$ for two extreme situations. There are two competing energies in the problem, the elastic energy and the impurity energy. If the impurity potential dominates, then we expect that the phase will adjust itself so that $QR_i + \phi(R_i) = -\pi$ at each impurity site. The system will gain the impurity pinning energy of $V_0\rho_0$ while paying an elastic energy per impurity of

$$E_{\text{elas}} \approx \frac{v^2}{4\pi v'} \frac{1}{n_i} n_i^2 = n_i v_F, \tag{2.6}$$

where $n_i = N_{\text{imp}}/L$ in the number of impurity per unit length. It is then natural to introduce the dimensionless parameter

$$\epsilon = V_0 \rho_0 / n_i v_F. \tag{2.7}$$

The strong pinning case discussed above corresponds to $\epsilon \gg 1$ and can be realized by either a strong impurity potential or a dilute impurity concentration. In the opposite limit $\epsilon \ll 1$ we expect the elastic energy to dominate. The phase $\phi_0(x)$ will be slowly varying and the individual terms in H' can be positive or negative. However, we shall apply the general argument due to Harris[17] to show that even in this case the phase ϕ_0 can distort to take advantage of fluctuations in the impurity distribution by breaking of the system into domains and again ϕ_0 is not small. It is now clear that ϵ forms the criterion separating two extreme cases which must be treated separately.

Let us write

$$\phi = \phi_0 + \psi \tag{2.8}$$

and expand $H_0 + H'$ to second order in ψ. The linear term in ψ gives the equation determining ϕ_0

$$\nabla^2 \phi_0 - V_0 \rho_0 \sum_i \sin[QR_i + \phi_0(R_i)]\, \delta(x - R_i) = 0 \tag{2.9}$$

and the dynamics is determined by the term quadratic in ψ. This leads us to define

$$\mathcal{H}_\psi = \pi v' \int dx \left[p^2 + \frac{1}{4\pi^2} \left(\frac{v}{v'} \right)^2 (\nabla\psi)^2 \right] + \frac{V_0\rho_0}{2} \sum_i \psi(R_i)^2 \cos[QR_i + \phi_0(R_i)]. \tag{2.10}$$

It is convenient to go to momentum space

$$\psi_q = \frac{1}{L} \int dx\, e^{iqx} \psi(x), \tag{2.11}$$

and

$$\mathcal{H}_\psi = \pi v' \sum_q \left[|p_q|^2 + \frac{1}{4\pi^2} \left(\frac{v}{v'} \right)^2 q^2 |\psi_q|^2 \right] - \tfrac{1}{2} V_0 \rho_0 \sum_{q,q'} \psi_q \psi_{q'} S(q + q'), \tag{2.12}$$

where

$$S(q) = \frac{1}{L} \sum_i e^{iqR_i} \cos[QR_i + \phi_0(R_i)]. \tag{2.13}$$

The dynamics of the phase mode are best described by the phase mode Green's function

$$\mathfrak{D}(q, q', i\omega_n) = \int_{-\beta}^{\beta} d\tau\, e^{i\omega_n \tau} \langle T \psi_q(\tau) \psi_{-q'}(0) \rangle. \tag{2.14}$$

From the equation of motion it is easy to show that

$$\mathfrak{D}(q,q',i\omega_n)=\delta_{q,q'}\mathfrak{D}_0(q,i\omega_n)+\tfrac{1}{2}V_0\rho_0\sum_{q''}\mathfrak{D}_0(q,i\omega_n)S(q''-q)\times\mathfrak{D}(q'',q',i\omega_n), \quad (2.15)$$

where

$$\mathfrak{D}_0(q,i\omega_n)=4\pi v'(\omega_n^2+v^2q^2)^{-1}, \quad (2.16)$$

is the unperturbed Green's function.

The goal of this paper is to solve Eq. (2.15) to obtain $\langle\mathfrak{D}(q,q',i\omega_n)\rangle_{\rm av}$ where $\langle\ \rangle_{\rm av}$ denoted averaging over impurities configurations. Furthermore starting from the phenomenological equation for the current carried by the CDW

$$J=\frac{e}{\pi}\int dx\,\dot{\phi}, \quad (2.17)$$

it is easy to show using Kubo's formula that the frequency-dependent conductivity is given by[12]

$$\sigma(\omega)=\frac{i\omega}{2}\left(\frac{e}{\pi}\right)^2 L\mathfrak{D}(0,0,i\omega_n\to\omega-i\delta). \quad (2.18)$$

In the next two sections we shall discuss the solution in the limits $\epsilon\gg1$ and $\epsilon\ll1$, respectively.

III. STRONG PINNING CASE ($\epsilon>>1$)

The limit is achieved by having either a strong impurity potential or by having a dilute impurity concentration. In this limit the impurity potential dominates and the CDW distorts to take maximal advantage of the impurity potential. The equilibrium configuration $\phi_0(x)$ is simply given by the relation $\cos[QR_i+\phi_0(R_i)]\approx-1$ and we have $S(q)=-L^{-1}\sum_i e^{iqR_i}$. The problem now reduces to a familiar one in random systems. The standard treatment of this problem is to introduce the self-energy function Γ

$$\langle\mathfrak{D}(q,q',i\omega_n)\rangle_{\rm av}=\delta_{q,q'}[\mathfrak{D}_0(q)^{-1}-\Gamma]^{-1}\equiv\delta_{q,q'}\mathfrak{D}(q,i\omega_n), \quad (3.1)$$

where Γ is given in the single-site t-matrix approximation as illustrated in Fig. 1.

$$\Gamma=n_i(-\tfrac{1}{2}V_0\rho_0)\left(1+\frac{V_0\rho_0}{2}A\right)^{-1}, \quad (3.2)$$

where

$$A=L^{-1}\sum_q\mathfrak{D}(q,i\omega_n)=2\pi\frac{v'}{v}(\omega_n^2-4\pi v'\Gamma)^{-1/2}. \quad (3.3)$$

The t-matrix approximation is lowest order in n_i and has ignored correlations between impurities. We shall return to discuss its validity later. With-

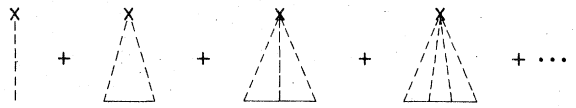

FIG. 1. Diagrams contributing to the self-energy Γ. Crosses represent the impurity potential and solid line is the phase phonon propagator.

in this approximation Γ must be solved self-consistently by combining Eqs. (3.2) and (3.3). It is convenient to define the frequency

$$\omega_0=n_iv \quad (3.4)$$

which is the frequency of a standing wave with wave vector equal to the inverse of the average spacing between impurities. Define the dimensionless quantities $\tilde{\omega}=\omega/\omega_0$ and $F=4\pi v'\Gamma/\omega_0^2$ and analytically continue $i\omega_n\to\omega-i\delta$, the self-consistency condition becomes

$$F=-2\pi\epsilon[1+\pi\epsilon(-\tilde{\omega}^2-F)^{-1/2}]^{-1}. \quad (3.5)$$

This is a cubic equation for F which can be solved. It is interesting to first consider the limit $\epsilon\to\infty$ in which case Eq. (3.5) becomes

$$F=-2(-\tilde{\omega}^2-F)^{1/2}. \quad (3.6)$$

The solution of this equation is simply that

$$F=-2-2(1-\tilde{\omega}^2)^{1/2}. \quad (3.7)$$

Substituting into Eq. (3.1) gives

$$\mathrm{Im}\mathfrak{D}(q=0,\omega-i\delta)=-\frac{8\pi v'}{\omega_0^2}\tilde{\omega}^{-4}(\tilde{\omega}^2-1)^{1/2},\quad \tilde{\omega}>1$$
$$=0\quad \tilde{\omega}<1, \quad (3.8)$$

This form of $\mathrm{Im}\mathfrak{D}$ satisfies the sum rule

$$\int_{-\infty}^{\infty}d\omega\,\omega\,\frac{\mathrm{Im}\mathfrak{D}}{4\pi v'}=\pi. \quad (3.9)$$

We recall from Eq. (2.18) that

$$\mathrm{Re}\sigma(\omega)=\frac{\omega}{2}\left(\frac{e}{\pi}\right)^2\mathrm{Im}\mathfrak{D}(q=0,\omega-i\delta). \quad (3.10)$$

In Fig. 2 we show plots for $\mathrm{Re}\sigma(\omega)$ for two values of ϵ. We note that $\mathrm{Re}\sigma(\omega)$ is relatively insensitive to ϵ as long as $\epsilon>1$ and that ω_0 is the characteristic energy at which $\mathrm{Re}\sigma(\omega)$ shows a peak. Thus the important contribution to the spectral weight arises from standing waves trapped between neighboring impurity sites. One might have expected to find a second class of mode in which a finite section of length n_i^{-1} oscillates about the harmonic potential due to a simple impurity potential. Such a mode will be expected to be at $(2\pi\epsilon)^{1/2}\omega_0$. Examination of our solution shows no particular feature in that frequency range. These modes are

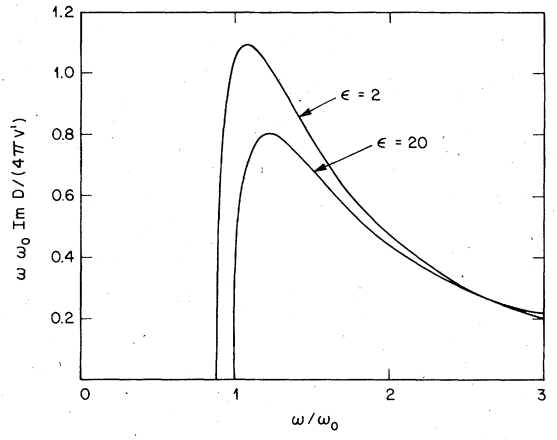

FIG. 2. Imaginary part of the phase correlation function vs ω/ω_0 for the strong pinning case for two different pinning parameters ϵ. This is related to the frequency-dependent conductivity by Eq. (2.18).

probably not important because for $\epsilon > 1$ the elastic energy is too small to sustain a rigid motion of a finite section of the CDW.

In the single-site t-matrix approximation $\mathrm{Re}\sigma(\omega)$ has a gap at $\omega \approx \omega_0$. Physically one expects to find spectral weight at lower frequency since there exist probabilities of finding two neighboring sites that are farther apart than the average spacing n_i^{-1}. The proper treatment of such low-frequency excitation is beyond the scope of the single-site approximation which we expect to be valid for $\omega \gtrsim \omega_0$. To estimate the spectral weight at lower frequencies we proceed as follows. The probability of finding two neighboring sites a given distance l apart is given by $n_i e^{-ln_i}$. In the limit $\epsilon \to \infty$ we simply assume a distribution of independent oscillators with frequencies given by $v(\pi/l)$. Their contribution to the spectral weight is approximately

$$\omega \mathrm{Im}\mathfrak{D}_0(q=0,\omega) \approx 4\pi v' \int_0^\infty dt\, e^{-t}\, \frac{\pi}{2}\, \delta\left(\omega - \frac{\pi v n_i}{t}\right) = 2\pi^3 v' \omega_0 e^{-\pi\omega_0/\omega}/\omega^2. \tag{3.11}$$

We note that the spectral weight is exponentially small for small ω. The easiest way of combining this low-frequency behavior with the high-frequency solution obtained earlier is to assume a Green's function of the form

$$\mathfrak{D}(q,\omega) = 4\pi v'[-\omega^2 + v^2q^2 - F - if(\omega)]^{-1}, \tag{3.12}$$

where

$$f(\omega) = \frac{\pi^2\omega_0}{2\omega^3}\, e^{-\pi\omega_0/\omega}\,[F(\omega=0)]^2, \tag{3.13}$$

is chosen to reproduce Eq. (3.11) in the limit $\omega \to 0$.

IV. WEAK PINNING CASE ($\epsilon \ll 1$)

The limit $\epsilon \ll 1$ applied when either the impurity potential is weak or the impurity concentration is dense. In this case $\phi_0(x)$ is slowly varying and at the impurity site the total phase $QR_i + \phi_0(R_i)$ is distributed almost randomly. Harris[17] has studied a similar problem for a magnetic system and has shown that this distribution is not completely random as the system can gain energy by taking advantage of the fluctuation in impurity distribution. We shall apply his arguments to the present problem. Let us assume that $\phi_0(x)$ varies on scale given by a length L_0. Within this length the total impurity potential has fluctuations of order $L_0^{1/2}$ and by adjusting ϕ_0 this potential energy can be gained. To estimate this gain in potential energy let us make the simplifying assumption that $\phi_0(x) = \bar{\phi}$ is constant within the length L_0. The impurity potential energy for the length L_0 is given by

$$V(L_0) = V_0\rho_0\, \mathrm{Re}\left(\sum_i{}' e^{i(QR_i+\bar{\phi})}\right), \tag{4.1}$$

where the sum is restricted to impurities within the length L_0 and on the average there are n_iL_0 terms in the sum. For $\epsilon \ll 1$, n_iL_0 is much greater than one and Eq. (4.1) can best be viewed as a random-walk problem in the two-dimensional complex plane. The radial distance in each step is unity and the angle is equal to QR_i which is random. It is clear that after n_iL_0 steps $\bar{\phi}$ can be chosen so that $V(L_0)$ takes on its minimum value given by

$$V_{\min}(L_0) = -V_0\rho_0\left\langle\left|\sum_i{}' e^{iQR_i}\right|\right\rangle_{\mathrm{av}} = -V_0\rho_0(n_iL_0)^{1/2}. \tag{4.2}$$

The second line in Eq. (4.2) follows from the following argument. Let

$$X_n = \sum_{i=1}^{n} e^{iQR_i},$$

then

$$\langle|X_{n+1}|^2 - |X_n|^2\rangle_{\mathrm{av}} = \langle|X_n + e^{iQR_{n+1}}|^2 - |X_n|^2\rangle_{\mathrm{av}} = 1 + 2X_n\langle\cos QR_{n+1}\rangle_{\mathrm{av}} = 1. \tag{4.3}$$

Thus we conclude that $\langle|X_n|^2\rangle_{\mathrm{av}} = n$ and if we make the reasonable assumption that $\langle|X_n|\rangle_{\mathrm{av}} = \langle|X_n|^2\rangle_{\mathrm{av}}^{1/2}$, Eq. (4.2) follows.

In order to take advantage of the potential energy in each section of length L_0 the phase must vary smoothly from section to section. The elastic energy required is estimated to be

$$K(L_0)=\frac{v_F}{4\pi}\int_0^{L_0}dx\,\langle|\nabla\phi_0|^2\rangle_{\rm av}=\frac{v_F}{4\pi}\,\frac{1}{\alpha L_0}\,, \tag{4.4}$$

where α is a numerical coefficient. If we further assume that the phase difference from section to section is random between $-\pi$ to π and that the true solution smoothly interpolates between them, this numerical factor can easily be determined to be

$$\alpha=3/\pi^2. \tag{4.5}$$

The characteristic length (or domain size) L_0 can now be determined by minimizing the total energy per unit length

$$E=L_0^{-1}[K(L_0)+V_{\rm min}(L_0)]. \tag{4.6}$$

The result is given by

$$L_0^{-1}=[(\alpha\pi V_0\rho_0/v_F)^2 n_i]^{1/3} \tag{4.7}$$

or the dimensionless combination

$$(n_iL_0)^{-1}=(\alpha\pi\epsilon)^{2/3}. \tag{4.8}$$

This confirms the physical picture that for $\epsilon\ll 1$, $\phi_0(x)$ varies slowly from one impurity site to the next and that a finite energy per unit length can be gained by properly distorting $\phi_0(x)$ to take advantage of the impurity potential.

We are now ready to solve Eq. (2.15) to obtain $\mathfrak{D}(q,\omega)$. Once again we formulate the problem in terms of the self-energy Γ as defined by Eq. (3.1). The novel feature is that the first-order term

$$\Gamma_1=\frac{V_0\rho_0}{2L}\sum_i\cos[QR_i+\phi_0(R_i)]\,, \tag{4.9}$$

which is usually assumed to vanish is in fact nonzero. Due to the sinusoidal nature of the CDW the restoring force has the same form as the impurity potential term $V(L_0)$ considered earlier. By dividing the chain into finite segments of length L_0, Γ_1 can be estimated using Eq. (4.2) as

$$\Gamma_1=-\tfrac{1}{2}V_0\rho_0(n_iL_0)^{1/2}/L_0. \tag{4.10}$$

To this order we obtain a pinning frequency given by

$$(-4\pi v'\Gamma_1)^{1/2}=2^{1/2}\alpha^{1/6}\gamma, \tag{4.11}$$

where we have found it convenient to introduce the frequency γ defined by

$$\gamma=\alpha^{-2/3}vL_0^{-1}, \tag{4.12}$$

where α is the numerical factor defined in Eq. (4.4). This frequency can be interpreted as the excitation of the phase mode with a wavelength of the order of the domain size L_0. In terms of the frequency scale $\omega_0=vn_i$ introduced earlier

$$\gamma=(\pi\epsilon)^{2/3}\omega_0. \tag{4.13}$$

It is now clear that the previous work of Fukuyama which performs an expansion in $\psi(x)$ and has ignored the Γ_1 term should be valid for $\omega\gtrsim\gamma$ (our γ is up to a numerical factor the same as the characteristic frequency obtained in that paper). This is because high-frequency excitations involve characteristic wavelengths that are short compared with L_0. In such cases an expansion in $\phi(x)$ is reasonable and the more subtle considerations here play no role. For $\omega<\gamma$ the previous work runs into problems with analyticity. As we shall show these difficulties are by and large removed by the present treatment.

We also note that Sokoloff[16] has argued that for weak impurity potential the CDW is not pinned. The reason given is that the pinning energy is of order $L^{1/2}$, where L is the size of the system whereas the force on the system due to the applied electric field is linear in L. What is wrong with this argument is now apparent since we have shown that the pinning energy is in fact proportional to L even though it is reduced by $(n_iL_0)^{-1/2}$ relative to the strong pinning case. In other words in Sokoloff's argument, L is limited to L_0 and is not permitted to go to infinity. Of course our conclusion is limited to the linear conductivity. Effects that are nonlinear in the electric field are beyond the scope of the present analysis.

The lowest-order contribution to Γ yields a δ-function spectrum for $\mathfrak{D}$. Fluctuations about this pinning frequency are included by going to higher orders in the expansion. The second-order contribution to Γ is given by

$$\Gamma_2=\left(\frac{V_0\rho_0}{2L}\right)^2\sum_{q\neq 0}\mathfrak{D}(q,\omega)\times\sum_{i\neq j}e^{iq(R_i-R_j)}\cos[QR_i+\phi_0(R_i)]\times\cos[QR_j+\phi_0(R_j)].$$

We note that the $q=0$ term is excluded in the q sum because its contribution is already included in Γ_1. It is clear that in the sum over i and j the $i\neq j$ terms have random phase and will cancel. Keeping only the $i=j$ term we obtain

$$\Gamma_2=(n_i/2)(V_0\rho_0/2)^2A, \tag{4.14}$$

where A is given by Eq. (3.3). This can also be written

$$4\pi v'\Gamma_2=-\gamma^3(-\omega^2-4\pi v'\Gamma)^{-1/2}. \tag{4.15}$$

If we set $\Gamma=0$ in Eq. (4.15) we recover the ω^{-1} divergence in the self-energy first noted by Lee, Rice, and Anderson. If we simply insert the first-order result $\Gamma=\Gamma_1$ in Eq. (4.15) this singularity is removed and we have

$$\mathfrak{D}_1(q,\omega)=\frac{4\pi v'}{-\omega^2+v^2q^2+2\alpha^{1/3}\gamma^2+\gamma^3(-\omega^2+2\alpha^{1/3}\gamma^2)^{-1/2}}\,. \tag{4.16}$$

The imaginary part of $\mathfrak{D}_1(q,\omega)$ shows a gap at $\omega=2^{1/2}\alpha^{1/6}\gamma$ which describes the existence of a pinned mode. It is interesting to note that for $\omega\ll\gamma$, the first- and second-order self-energy corrections shown in Eq. (4.16) are in fact the same order in γ [or using Eq. (4.13), the same order in ϵ]. However, Eq. (4.16) is still unsatisfactory as a pole exists in the upper half plane of $\mathfrak{D}_1(q,\omega)$. As a result the Kramers-Kronig relation is not obeyed and the sum rule given in Eq. (3.9) is off by a factor of 3. The situation can be remedied by requiring Γ to be self-consistent. The self-consistency equation is obtained by combining Eqs. (4.11) and (4.15)

$$\Gamma=-2\alpha^{1/3}\gamma^2+\gamma^3(-\omega^2-4\pi v'\Gamma)^{-1/2}. \tag{4.17}$$

It is convenient to measure frequency in units of γ and introduce the following dimensionless quantities,

$$y=\omega/\gamma, \tag{4.18}$$

$$G=4\pi v'\Gamma/\gamma^2. \tag{4.19}$$

Then Eq. (4.17) becomes

$$G=-2\alpha^{1/3}+(-y^2-G)^{-1/2}. \tag{4.20}$$

Note that in the scaled variable the self-consistency equation is now independent of ϵ, and this is the consequence of the observation made earlier that the first- and second-order terms in Γ are the same order in ϵ. It is in fact possible to sum the series shown in Fig. 1 to all orders as done by Fukuyama,[12] the only modification being the nonvanishing of the first order term. It is easy to show that in the scaled variable the higher-order terms are higher order in ϵ. We have chosen for simplicity to treat here the $\epsilon\ll1$ limit and keep only the second-order term.

The Green's function is given by

$$\mathfrak{D}(q=0,\omega)=(4\pi v'/\gamma^2)[1/(-y^2-G)], \tag{4.21}$$

where G is obtained from Eq. (4.20) by solving a cubic equation. The result for $\mathrm{Re}\sigma(\omega)$ is shown in Fig. 3. While a peak occurs around $y\approx1$ or $\omega\simeq\gamma$ as expected this result for $\sigma(\omega)$ is still unsatisfactory. We find that for small ω, $\mathrm{Re}\sigma(\omega)\sim|\omega|$. This implies that the Kramers-Kronig relation is not obeyed because that requires that $\mathrm{Im}\sigma(\omega\to0)\sim\omega\ln\omega$ which is not the case. The source of this difficulty can be traced back to the fact that for $y=0, G(y=0)$ obtained from Eq. (4.20) is complex and hence $\mathrm{Im}\mathfrak{D}(q=0,\omega\to0)$ is nonzero. It is easy to show from Eq. (4.20) that the condition for

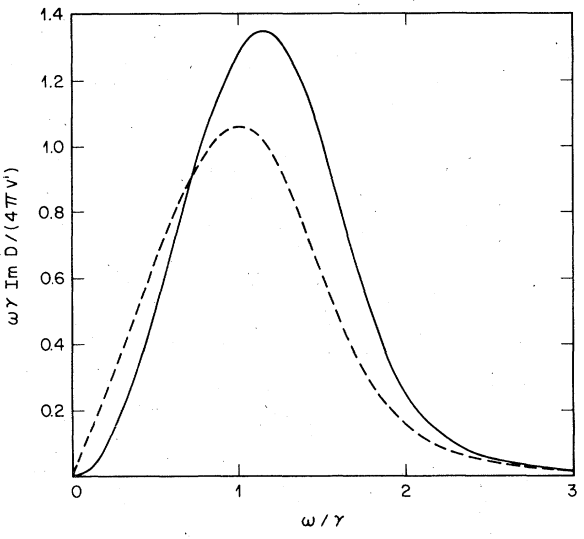

FIG. 3. Imaginary part of the phase correlation function vs ω/γ for the weak pinning case. Solid line corresponds to the choice of $2\alpha^{1/3}=3\times2^{-2/3}$ and satisfies the sum rule. Dashed line corresponds to $\alpha=3/\pi^2$. Note the linear behavior for small ω. The dashed line does not satisfy the sum rule.

$G(y=0)$ to be real is that

$$2\alpha^{1/3}\geq3\times2^{-2/3}=1.89. \tag{4.21a}$$

With our choice of α given in Eq. (4.5), $2\alpha^{1/3}=1.345$ and this inequality is not obeyed. We note that this choice of α is based on rather crude estimates of the minimization of the total energy. We therefore take the point of view that α should be adjusted to obtain a result that has the proper analytic properties. It is possible to show directly that if α is chosen to obey Eq. (4.21) then the sum rule Eq. (3.9) is satisfied. We also note that if α is chosen to satisfy the equality in Eq. (4.21), $\sigma(\omega)\sim\omega^2$ for small ω; otherwise a gap exists in the spectral weight. We feel that a reasonable approximate solution is obtained by choosing $2\alpha^{1/3}=1.89$. The result is shown in Fig. 3.

Finally we remark on the static dielectric constant ϵ_0 which is directly related to the real part of $\mathfrak{D}(0,0)$. This has the form

$$\epsilon_0=c(\omega_p/\gamma)^2, \tag{4.22}$$

where $\omega_p^2=4\pi ne^2/m^*$. The numerical coefficient depends on the choice of α and for $2\alpha^{1/3}=1.89$, $c=1.59$. The functional form of Eq. (4.22) is independent of α and has the satisfactory interpretation of being the contribution to the dielectric constant due to the pinned mode at a characteristic frequency γ given by Eq. (4.13).

V. CONCLUSION

In this paper we have studied the effect of impurities on the dynamics of the charge-density wave. We have restricted our attention to phase fluctuations only and our conclusions should be valid at low temperatures. We distinguish between the strong and weak pinning regimes. When the impurities are either dilute or their coupling to the charge-density wave strong, it is physically obvious that pinning will occur. In this limit we obtain an analytic form for the dynamic response function. On the other hand, when the impurities are dense or their coupling weak, the pinning effect is much more subtle. We find that in this case the system can be thought to break up into domains whose size we can estimate. The domain size also determines the pinning frequency which is found to go as the one-third power of the impurity concentration. The response function and the frequency-dependent conductivity are also calculated in this limit.

While we have restricted our attention to one-dimensional systems in this paper, the general consideration can also be applied to higher dimensions. In particular, the layered compounds[18] are very interesting experimental systems to study. In the weak pinning case we can apply similar arguments as those made in Sec. IV. Let the elastic energy be given by $\frac{1}{2}K\int d^2x\,(\nabla\phi)^2$ and let n denote the two-dimensional impurity concentration. It is easy to show that the domain size L_0 is given by

$$L_0^{-1} \approx (V_0\rho_0/K)n^{1/2}.$$

Furthermore the pinning frequency should again be given by vL_0^{-1}. This result is different from that of McMillan,[19] who found a pinning frequency which goes as $n^{1/4}$. The difference arises from the fact that McMillan has factorized the quartic term in the free energy into quadratic terms which he then treates self-consistently. While the charge-density wave is permitted to adjust to the impurity potential, both amplitude and phase fluctuations are equally likely in his treatment. We feel that our treatment is more realistic in the low-temperature limit.

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