Domain motion and threshold behavior of charge-density waves

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The relationship between the various computer-simulation theories of charge-density-wave motion is discussed, and some new simulation results in one and three dimensions are presented, which provide evidence that the motion near threshold proceeds by domains analogous to the Lee-Rice domains becoming unstable and jumping rapidly. The consequences of a model based on this picture are then discussed. This model leads to a threshold field which is different from the Lee-Rice depinning field (which is argued to be the field necessary to depin a typical domain but not necessarily sufficient to cause sustained motion of the charge-density wave), for strong pinning.

I. INTRODUCTION

In recent years, the realization of Fröhlich conductivity,[1] i.e., electrical conduction due to the motion of a charge-density wave, has been discovered in $NbSe_3$, TaS_3, and several other compounds.[2] Although such systems are not superconductors (as it was originally thought that Fröhlich conductors would have high conductivity), they exhibit interesting nonlinear conduction and an interesting noise spectrum above a well-defined dc threshold electric field. Theories of Fröhlich conduction are of two types: classical models, in which classical equations of motion of the charge-density wave are solved,[3–10] and quantum-mechanical models,[11] in which a macroscopic chunk of the charge-density wave tunnels through a potential barrier. Aside from the trivial single-particle classical model,[3] which can be solved exactly, nontrivial models, i.e., models in which internal distortions of the charge-density wave are taken into account, have only been solved analytically near threshold in mean-field theory[5] which is valid in four or more dimensions. Far above threshold, perturbation theory has been done to lowest two orders in powers of the reciprocal of the applied field.[8] Even in this order, evidence of nonlinearity has been found. Fisher has devised a scaling theory based on this perturbation theory and has stressed an analogy of the threshold behavior of a charge-density wave to critical phenomena.[5] The only nonperturbative methods valid near threshold have been computer simulations, done primarily on one-dimensional systems.[9,10,12]

Computer simulations have been done on both models in which a rigid charge-density wave interacts with a distortable lattice containing random substitutional impurities[9,10] and on a model based on the Fukuyama-Lee model,[6,12] in which the lattice is rigid and the charge-density wave distorts. The two models are shown in Sec. II to be equivalent, and the question of whether the charge-density wave or the lattice distorts more is discussed. Computer simulations performed on both the one-dimensional and three-dimensional models are reported in Sec. III and give evidence that just above threshold, motion occurs by Lee-Rice-like domains becoming unstable and moving, followed by other domains becoming unstable at other points in the crystal, etc.

An argument is given to show that in greater than two dimensions, a model in which the motion occurs adiabatically at slow speed (i.e., by taking an equilibrium configuration solution and translating the origin by Vt, where V is an average center of mass velocity) will have a zero dynamical threshold field (i.e., the value of the applied field below which motion ceases). Since the molecular-dynamical calculations show that the motion occurs by nonadiabatic motion, a model based on the unstable domain picture is used to calculate the dependence of the threshold field on the impurity potential strength. The expression found is different from the Lee-Rice field, for strong pinning.

II. MODELS FOR COMPUTER SIMULATIONS

In this section, the relationships between the various models for computer simulations of sliding charge-density waves are discussed. Some computer simulations are based on discretized versions of the one-dimensional Fukuyama-Lee model,[12] and some are based on a rigid charge-density-wave model.[9,10] We shall see, however, that the two approaches lead to similar models. The hope is that one-dimensional models are sufficient to give much of the physics of the problem.

In the Fukuyama-Lee model,[6] the charge-density wave is assumed to produce a charge density given by

$$\rho_0 \cos[Qx+\phi(x)] , \tag{1}$$

where Q is the wave vector of the charge-density wave, ρ_0 is the amplitude, which is assumed to be constant, and $\phi(x)$ is the phase, which is assumed to vary slowly over a distance comparable to the range of the impurity potential. Under these circumstances, if $V(x-x_j)$ is the potential due to an impurity located at site x_j, the interaction with the impurity is given by

$$\rho_0 \int dx\, V(x-x_j)\cos[Qx+\phi(x)] \approx \rho_0 v(Q)\cos[Qx_j+\phi(x_j)] , \tag{2}$$

where $v(Q)$ is the Fourier transform of $V(x)$. To treat the distortion of the charge density wave, the phase is treated as an elastic medium. Then, the total energy of

the system is given by

$$\int dx \left[\alpha \left(\frac{\partial \phi}{\partial x} \right)^2 + \sum_j v(Q)\cos[Qx+\phi(x)]\delta(x-x_j) - Fx \right] , \quad (3)$$

where j is summed over impurity sites, F is an external field, and α is the force constant. Most models assume that when the charge-density wave is moving, there is a damping force due to the excitation of electronic excitations and that this damping force dominates over the inertial term, which is neglected. The justification for this is that optical experiments show that the zero-wave-vector phason mode is overdamped.[13] Pietronero and Strassler,[12] in order to simplify the equations of motion, assume that the damping force only acts at the impurity positions. That is, they write their damping-force density as

$$-\gamma \sum_j \dot{\phi}(x)\delta(x-x_j) , \quad (4)$$

where γ is a constant. They obtain the equation of steady-state motion by setting the damping-force density plus the negative of the derivative of the energy density with respect to $\phi(x)$ equal to zero. This gives

$$\gamma \sum_j \dot{\phi}(x)\delta(x-x_j) = -\alpha \frac{\partial^2 \phi}{\partial x^2} - v(Q) \sum_j \cos[Qx+\phi(x_j)]\delta(x-x_j) . \quad (5)$$

Between impurity sites Eq. (5) reduces to

$$-\alpha \frac{\partial^2 \phi}{\partial x^2} + F = 0 , \quad (6)$$

which is trivially integrated to yield

$$\phi(x) = \frac{1}{2}\frac{F}{\alpha}x^2 + \left[-\frac{1}{2}\frac{F}{\alpha}(x_j + x_{j-1}) + \frac{\phi(x_j)-\phi(x_{j-1})}{x_j - x_{j-1}} \right] x + C \quad (7)$$

for $x_{j-1} < x < x_j$, where C is an arbitrary constant. If we integrate Eq. (5) from $x_{j-1}+\epsilon$ to $x_{j+1}-\epsilon$ where ϵ is a small number and substitute for the value of $\partial\phi/\partial x$ using Eq. (7), we obtain

$$\gamma \dot{\phi}_j = +\alpha \left[\frac{\phi(x_{j+1})-\phi(x_j)}{x_{j+1}-x_j} - \frac{\phi(x_j)-\phi(x_{j-1})}{x_j - x_{j-1}} \right] - Qv(Q)\sin[Qx_j+\phi(x_j)] + \frac{1}{2}\frac{F}{\alpha}(x_{j+1}-x_{j-1}) . \quad (8)$$

This is the model first introduced by Teranishi and Kubo[12] and is the starting point for Pietronero and Strassler's calculations. We can also treat the case of substitutional impurities in a periodic lattice by substituting ja, where a is the lattice constant, for x_j in Eqs. (2)—(4) and replacing $v(Q)$ by $v(Q)c_j$ in Eq. (2), where c_j has one value on an impurity site and a different value on a nonimpurity site. If we neglect the lattice potential and consider only the impurity potential, $c_j = 1$ on an impurity site and zero otherwise. Then, Eq. (8) becomes

$$\dot{\phi}_j = -\frac{\alpha}{a\gamma}(2\phi_j - \phi_{j+1} - \phi_{j-1}) - \frac{Qv(Q)}{\gamma} c_j \sin(Qaj + \phi_j) + \frac{Fa}{\gamma\alpha} , \quad (9)$$

where $\phi_j = \phi(ja)$. Equation (9) is identical to the model used in Refs. 9 and 10, even though in those references it was assumed that the charge-density wave was rigid but the lattice distorted so that the wave could accommodate the impurities, which is the opposite of what was assumed in deriving Eq. (9). Therefore, it appears that whether it is the lattice, the charge-density wave or both which distort, all the models that have been used in molecular-dynamical calculations describe all of these possibilities.

Actually, the experimental results of Ong and Maki[14] favor a model in which the charge-density wave is quite rigid, whereas most workers in the field assume that the lattice is rigid and the wave distorts. In order to determine which picture is more correct, we will estimate an effective force constant for the phason mode and compare it to that for the lattice. This can be done using the work of Lee, Rice, and Anderson.[15] The effective force constant K is defined by

$$\omega^2 = V_F^2 \frac{m}{m^*} q^2 = \frac{K}{m^*} , \quad (10)$$

where m and m^* are the electron mass and the effective mass for the phason and V_F is the Fermi velocity. Then, taking

$$\omega^2 = c^2 q^2 = \frac{K'}{M} \quad (11)$$

for the phonons, where M is an ionic mass and c is the phonon velocity, we obtain

$$\frac{K}{K'} = \frac{V_F^2}{c^2}\frac{m}{M} . \quad (12)$$

Taking $V_F \sim 10^7$ cm/s, $c \sim 10^4$ cm/s, and $M/m \sim 10^3$ we obtain

$$\frac{K}{K'} \sim 10^3 ,$$

which favors the stiff charge-density-wave model.

If we set $c_j \equiv 1$, Eq. (9) is just the pure Frankel-Kontorova model.[10,16] As in Ref. 16, it was found useful to study the lattice dynamics of these models when near threshold. As in the case of the incommensurate Frankel-Kontorova model, the low frequency modes will be found to be highly localized for fields near threshold and the lowest mode will become unstable. The localization length for the lowest frequency modes must be of the order of the relevant domains in the problem (perhaps the Lee-Rice domains). In order to study the vibrational modes we replace $\phi(x)$ by $\phi_0(x)+\delta\phi(x)$ in Eq. (5), where $\phi_0(x)$ is an equilibrium solution to Eq. (5), and linearize in $\delta\phi$. Using Eq. (5), we obtain

$$\sum_j \gamma\delta\dot{\phi}(x)\delta(x-x_j)$$
$$=-\alpha\frac{\partial^2\delta\phi}{\partial x^2}-Qv(Q)\sum_j c_j\sin[Qx_j+\phi_0(x_j)]\delta(x-x_j)\ . \tag{13}$$

Applying the procedures in Eqs. (5)—(7) to Eq. (13), we find

$$\delta\dot{\phi}_j=-\frac{\alpha}{a\gamma}(2\delta\phi_j-\delta\phi_{j+1}-\delta\phi_{j-1})$$
$$-Q^2\gamma^{-1}v(Q)c_j\cos(Qja+\phi_{0j})\delta\phi_j\ . \tag{14}$$

Diagonalizing Eq. (14) gives the relaxation mode decay constants (i.e., the squares of the phonon frequencies). When one of these decay constants becomes negative (i.e., the frequency becomes imaginary), that mode will grow instead of decaying, signifying the situation in which a domain becomes depinned.

A natural generalization of Eq. (9) to three dimensions is

$$\dot{\phi}_{jkl}=-\frac{\alpha}{a\gamma}(6\phi_{jkl}-\phi_{j+1,k,l}-\phi_{j-1,k,l}$$
$$-\phi_{j,k+1,l}-\phi_{j,k-1,l}-\phi_{j,k,l+1}-\phi_{j,k,l-1})$$
$$-\frac{v(Q)}{\gamma}Qc_{jkl}\sin(Qja+\phi_{jkl})+\frac{Fa}{\gamma\alpha}\ . \tag{15}$$

Here j,k,l label the lattice vectors [i.e., $R_{jkl}=(j,k,l)a$], and $c_{jkl}=1$ only on impurity sites and is zero otherwise. Although the computational time could be reduced considerably if we generalized Eq. (8) to three dimensions instead, its generalization has a volume instead of a length multiplying F, and this volume is not easy to determine for general impurity configurations.

III. COMPUTER-SIMULATION RESULTS FOR UNSTABLE DOMAINS

In Ref. 9, it was postulated that at threshold for sliding, a phonon mode in a charge-density-wave system becomes unstable. Previous computer-simulation results on the pure incommensurate Frankel-Kontorova model for the case of a strong sinusoidal potential have shown that such a picture also holds for this model.[16] The unstable phonon mode was found to be highly localized. This suggests a picture of sliding near threshold in which a small localized region of the system becomes unstable and jumps to a new configuration. Computer simulations will be presented in order to verify that this picture also holds for the problem of a charge-density wave interacting with impurities. It appears to be reasonable to associate these unstable regions with the Lee-Rice domains that have been discussed by many workers. These calculations were performed for the substitutional impurity model given by Eq. (9) because the lattice vibrations are then easily determined using Eq. (14).

The following procedure was used. First the equilibrium configuration in zero applied field was determined by integrating Eq. (9) numerically, as has been done by the author in previous work. The external field was then increased to a point just below threshold. After the system reached an equilibrium configuration for a field just below the sliding threshold, Eq. (14) was diagonalized to find the lattice vibrations. As the field approached threshold, the lowest phonon mode frequencies decreased, and the lowest mode appeared to drop to zero frequency as threshold was approached. The lowest phonon mode eigenvectors are plotted in Fig. 1. It should be noted that the modes are localized. The degree of localization did not appear to change significantly as the threshold field was approached. The occurrence of a localized mode which goes unstable near threshold is like that found for the pure Frankel-Kontorova model.[16] The field was then raised slightly above threshold. The motion was found to proceed by a region whose size was of the order of the spatial extent of the lowest phonon mode eigenvector, becoming unstable and jumping to a new configuration. The process then repeats itself for another region in the crystal. This is similar to the behavior found previously[9] except that here the phonon modes were calculated for comparison. These calculations were performed for a 100-atom lattice containing 20 impurities. The ratio of the impurity potential to αa in Eq. (9) was taken to be 0.01. If we apply Fukuyama and Lee's formula for the domain size, we obtain in terms of the notation of this paper

$$\frac{L_0}{ca}=\left[\frac{4\pi^2}{3}\frac{\alpha c}{av(Q)}\right]^{2/3}, \tag{16}$$

where c is the impurity concentration. Using the values for the parameters in the calculations reported here, we find that the Fukuyama-Lee domain size is about 200 lattice constants. The actual domain size, however, was found to be about 20 lattice constants, as seen in Fig. 1. Similar molecular-dynamical runs were also made for $v(Q)/\alpha a$ equal to 0.1. In this case, the size of the unstable domain was found to be around 5 lattice constants, whereas the value found for the Fukuyama-Lee formula was found to be about 41.6. Thus these domain sizes appear to be proportional to the Lee-Rice domain sizes, al-

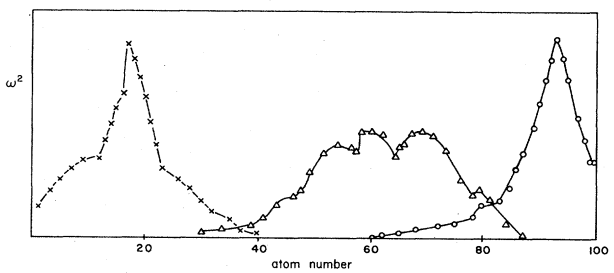

FIG. 1. The lowest three phonon eigenvectors are shown for a one-dimensional charge-density-wave model in a 100-atom lattice with 20 random substitutional impurities, for impurity potential $V/\alpha a=0.01$, and applied field $F/\alpha=0.007\,85$ (just below threshold). The modes shown have ○, $\omega^2=0.007\,75\alpha$; ×, $\omega^2=0.0124$; △, $\omega^2=0.0220$. The horizontal axis labels the atoms along the chain.

though the Lee-Rice domain sizes found for their formula are much larger.

Molecular-dynamical calculations were also done on the three-dimensional model described by Eq. (15). The sample size in these runs was $7\times7\times7$ atoms with 120 impurities distributed at random. As with the one-dimensional system, the equilibrium configuration in zero field was first found by integrating Eq. (15). Runs were then made with an applied field and the field was increased until a point slightly above threshold was reached. In this run $v(Q)/\alpha a$ was chosen to be 0.6, as smaller values gave domains which were larger than the sample size. It should be noted that the three-dimensional system is much stiffer than the one-dimensional system since for the one-dimensional system $v(Q)/\alpha a$ equal to 0.1 gave domain lengths of the same order of magnitude. This is expected because the Lee-Rice domain length is proportional to $[\alpha a/v(Q)]^{2/(4-d)}$ and hence we expect the domain length to be much larger for a given value of $v(Q)/\alpha a$ in three dimensions than in one dimension. The unstable domain structure found right above threshold in this three-dimensional calculation is shown in Fig. 2. Thus the picture of motion occurring by successive localized domains becoming unstable right near threshold appears to hold in three dimensions. Lattice dynamical calculations were not done for the three-dimensional system. Since the domains in these calculations are only a few atoms in size, it is difficult to determine whether the picture of large well-defined domains found in the one-dimensional model for much weaker impurity potential persists for the three-dimensional case. To ascertain this it would be necessary to repeat these calculations on much larger systems for a smaller value of $v(Q)/\alpha a$.

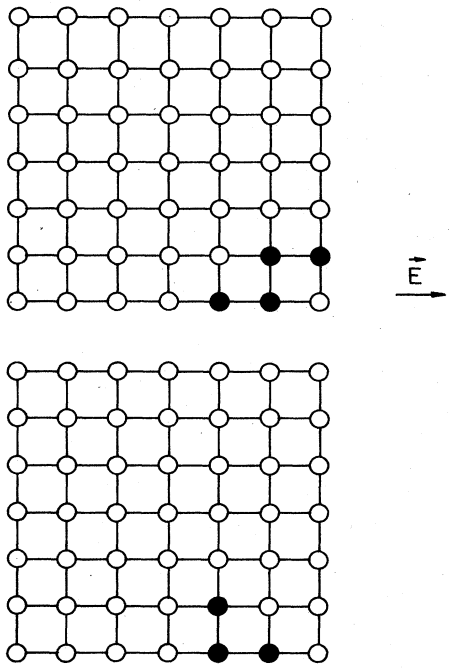

FIG. 2. Domain motion just above threshold for the three-dimensional model. The second and third atomic layers from the bottom of a $7\times7\times7$ crystal. The circles denote atomic positions. The shaded circles are sites at which the charge in the phase which occurs during a time equal to 0.2 of the decay time constant γ^{-1}. The direction of the applied field is indicated.

IV. THE DYNAMICAL THRESHOLD FIELD AND DOMAIN MOTION NEAR THRESHOLD

In Ref. 9, it was argued that the motion of a charge-density wave near the threshold for sliding could be characterized by the occurrence of quasistable vibrational modes. These modes are unstable, and hence grow exponentially with time, but the growth exponents are very small, and hence the system can remain in an unstable configuration for a long time. The growth exponents were found to be proportional to the square root of the difference between the applied field and a threshold field at which this mode becomes unstable. This result was then used to argue that the mean charge-density-wave current should have a square-root dependence on the difference between the applied and threshold fields for a finite system. The argument could be applied to a finite system, where there is only one unstable mode near threshold, but not for an infinite system where there could be an infinite number of such modes.

The molecular-dynamical calculations presented in Sec. III of this paper showed that these modes are highly localized and play the role ascribed to the Lee-Rice domains by many of the workers in the field. The calculations also showed that it was possible for one domain to become unstable and jump to a new configuration without the occurrence of sustained charge-density-wave motion. For such a case the unstable domain argument discussed in the preceding paragraph would not be expected to tell us anything about sustained charge-density-wave motion. The threshold field for the instability of a typical domain should be identified with the Lee-Rice depinning field. Thus it appears that there exists another threshold field, the dynamical threshold field, above which the applied field does enough work on the charge-density wave to overcome the energy lost due to the creation of internal vibrational excitations and the phenomenological damping-force term in the equations of motion. An applied field below this value is not able to sustain the motion.

The treatment of the dynamical threshold field presented here is essentially an extension of the procedure used in Ref. 17. That is, the mean work per lattice site done by the external field, $\mathbf{F}\cdot\mathbf{V}$, where $\mathbf{F}$ is the external field [which must be equal to Fa in Eq. (15)] and $\mathbf{V}$ is the mean center-of-mass velocity of the system, is set equal to the mean rate at which work is done by the impurity and/or lattice potentials in creating internal vibrational excitations of the system and the phenomenological damping term. Let us transform Eq. (15) to a Galilean reference frame in which the charge-density-wave center of mass is stationary on the average (i.e., a frame moving with velocity $\mathbf{V}$ relative to the old frame). This simply adds a term $-QVt$ to the argument of the sine and a constant $-\gamma V$ to the right-hand side of Eq. (15). Then, we have

$$\mathbf{F}\cdot\mathbf{V}=\frac{1}{T}\int_{-T/2}^{T/2}dt\sum_{j,k,l}\langle\dot{\phi}(\mathbf{R}_{j,k,l})v(Q)C_{j,k,l}\times\sin[Qja+\phi(\mathbf{R}_{j,k,l})-Qvt]\rangle+\gamma V^2\,, \tag{17}$$

where $\langle\ \rangle$ denotes an impurity average and T is some long time over which the averages are taken. For high-velocity motion, we neglect $\phi(\mathbf{R}_{j,k,l})$ in the argument of the sine in this equation, and we get a result which is equivalent to the zero-temperature limit of the result of Ref. 17 for the frictional force for the case in which the system is overdamped. [If the damping term were not included in Eq. (15) but the inertial term was, we would have precisely the results of Ref. 17.] The first term on the right-hand side of Eq. (17) is in this case simply the rate at which work is done on a collection of overdamped harmonic oscillators (i.e., the internal vibrations of the system) by the impurities. Substituting for $\dot{\phi}$ from Eq. (15) and carrying out the averages, we obtain

$$\mathbf{F}\cdot\mathbf{V}=\frac{c}{2}[v(Q)]^2\frac{1}{N}\times\sum_{\mathbf{k}}\mathrm{Im}\left[\frac{VQ}{-V^2Q^2+\omega_0^2(\mathbf{k})-i\gamma VQ}\right]+\gamma V^2\,, \tag{18}$$

where c is the impurity concentration, and $\omega_0(\mathbf{k})$ is the frequency of the phonon mode whose polarization is along $\mathbf{Q}$. Using the Debye model to do the summation over $\mathbf{k}$ in Eq. (18), we obtain

$$\mathbf{F}=\frac{3}{32\sqrt{2}}c\frac{[v(Q)]^2}{\omega_0^3}\gamma^{1/2}Q^{3/2}V^{1/2}+\gamma V\,, \tag{19}$$

where ω_0 is the Debye frequency for the phonon mode polarized along $\mathbf{Q}$. Using the fact that the first term on the right-hand side is much smaller than the second, we may solve this equation for V to lowest order in F to obtain precisely the result found by Sneddon, Cross, and Fisher,[8] which indicates that their work is equivalent to applying the methods of Ref. 17 to a system in which the phonons are overdamped (or at least the long-wavelength ones are). Since this result gives $F=0$ when $V=0$, implying zero dynamical threshold field, it cannot be correct near threshold. Of course, we expect the approximation of neglecting ϕ in the argument of the sine to break down near threshold because, as we have seen in Sec. III, ϕ can undergo quite large motion there. Therefore, a way must be found to include ϕ in the argument of the sine.

It can be shown that an adiabatic approximation[18] for ϕ cannot be correct because it results in a zero dynamical threshold field. An adiabatic approximation means that

$$\phi(\mathbf{r})=f(\mathbf{r}-\mathbf{V}t)\,, \tag{20}$$

where $f(\mathbf{r})$ is the solution to the equilibrium equations for ϕ for fields just below threshold. The physical reason why such a solution cannot give a nonzero threshold field is that if this solution is substituted in the argument of the sine in Eq. (17), the argument of the sine will cease to depend on time as V approaches zero. Since the first term on the right-hand side of this equation is the work done on a collection of driven harmonic oscillators (i.e., phonons), the driving term will only be able to excite zero frequency vibrations as V approaches zero. Since in three or more dimensions the phonon density of states goes to zero at least as the square of the frequency at zero frequency, the force F, given by Eq. (17), must vanish as V approaches zero. Sneddon has presented a solution of the form of Eq. (20) for the pure Frenkel-Kantorova model, however.[19]

To be more precise, if $\phi(\mathbf{r},t)$ only depends on $\mathbf{r}$ and t in the combination $\mathbf{r}-\mathbf{V}t$, the sine term on the right-hand side of Eq. (15) can be written as

$$\sin[\mathbf{Q}\cdot\mathbf{R}_\alpha+\phi(\mathbf{R}_\alpha-\mathbf{V}t)-\mathbf{Q}\cdot\mathbf{V}t]=\sum_{\mathbf{k}}A(\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{R}_\alpha-\mathbf{V}t)}\,, \tag{21}$$

where α denotes the indices j,k,l and $A(\mathbf{k})$ is the spatial Fourier transform of the sine on the left-hand side. Then, the time Fourier transform of this equation is

$$B(\omega)=\sum_{\mathbf{k}}A(\mathbf{k})\,|_{\mathbf{k}\cdot\mathbf{V}=\omega}\,. \tag{22}$$

Since the sine term is a finite quantity (at worst it has step-function-like singularities, as was shown to occur for the Frenkel-Kontorova model[20]), $A(\mathbf{k})$ must decay to zero for large $\mathbf{k}$. Then as V approaches zero, the range of frequencies for which $B(\omega)$ is large shrinks to zero [because of the restriction $\mathbf{k}\cdot\mathbf{V}=\omega$ on the summation over $\mathbf{k}$ in Eq. (22)]. If we substitute for $\dot{\phi}$ in Eq. (17) using Eq. (15) and use Eq. (21) to substitute for the sine terms, we obtain

$$\mathbf{F}\cdot\mathbf{V}=\frac{3}{32}\frac{C}{V_2}\frac{[v(Q)]^2}{\omega_0^3}\int d\omega\,B(\omega)\gamma^{1/2}\omega^{3/2}\,. \tag{23}$$

Since $A(\mathbf{k})$ falls off with increasing k at least as k^{-1} (the behavior for a step function), $|B(\omega)|^2$ converges when integrated over all ω. Since we have just argued that the width of $B(\omega)$ approaches zero linearly with V, we find from Eq. (23) that F approaches zero as V approaches zero, implying that dynamical threshold field is zero.

In order to have a nonzero dynamical threshold field, the system must exhibit local motion which does not cease in the limit as V approaches zero. A clue to this motion is given by the molecular-dynamical calculations reported in this paper and in previous work.[9] They show that motion just above threshold consists of domains becoming unstable and jumping to a new configuration, with most of the system remaining in its original configuration. This is then followed by another domain jumping to a new configuration, etc. The local velocities occurring during such a jump are not extremely rapid, as the term "jump" would imply, but they do not scale to zero as V approaches zero, as would occur in the adiabatic approximation solution. Then, a model suggested by the molecular-dynamical calculations is the following: Let

$$\phi(\mathbf{R}_\alpha,t)=\phi_0(\mathbf{R}_\alpha)+\sum_p g_p(\mathbf{R}_\alpha,\mathbf{R}_p,t-t_p)\,, \tag{24}$$

where $\phi_0(\mathbf{R}_\alpha)$ is the value of the phase before a time interval of length T running from $t=-T/2$ to $T/2$ and the function g approaches zero for $|\mathbf{R}-\mathbf{R}_p|\to\infty$. Here α is short-hand notation for (j,k,l). The g's describe the hopping domains and we take $-T/2<t_p<T/2$. We will assume that $g(\mathbf{R}_\alpha,\mathbf{R}_p,t-t_p)$ is only nonzero for one value of p, for a given choice of $\mathbf{R}_\alpha$ and t. Then we have

$$\sin[\mathbf{Q}\cdot\mathbf{R}_\alpha+\phi(\mathbf{R}_\alpha,t)+\mathbf{Q}\cdot\mathbf{V}t] \cong\sin[\mathbf{Q}\cdot\mathbf{R}_\alpha+\phi_0(\mathbf{R}_\alpha)+\mathbf{Q}\cdot\mathbf{V}t]+\sum_p f_p(\mathbf{R}_\alpha,\mathbf{R}_p,t-t_p)\ , \tag{25}$$

where

$$f_p(\mathbf{R}_\alpha,\mathbf{R}_p,t-t_p)=\sin[\mathbf{Q}\cdot\mathbf{R}_\alpha+\phi_p(\mathbf{R}_\alpha)+\mathbf{V}\cdot\mathbf{Q}t +g_p(\mathbf{R}_\alpha,\mathbf{R}_p,t-t_p)] -\sin[\mathbf{Q}\cdot\mathbf{R}_\alpha+\phi_p(\mathbf{R}_\alpha)+\mathbf{Q}\cdot\mathbf{V}t]\ , \tag{26}$$

where

$$\phi_p(\mathbf{R}_\alpha)=\phi_0(\mathbf{R}_\alpha)+\sum_{p'<p} g_{p'}(\mathbf{R}_\alpha,\mathbf{R}_{p'},\infty)\ .$$

We will now work out the consequences of this model. Substituting into Eq. (17) for $\dot\phi$ from Eq. (17) (and since we are interested in lowest order in the impurity concentration, we replace $c_\alpha c_\beta$ by $c\delta_{\alpha\beta}$), we obtain

$$\mathbf{F}\cdot\mathbf{V}=\frac{1}{TN}c\sum_\alpha |v(\mathbf{Q})|^2\int_{-T/2}^{T/2}dt\int_{-\infty}^{\infty}dt'\sin[\mathbf{Q}\cdot\mathbf{R}_\alpha+\phi(\mathbf{R}_\alpha,t)+\mathbf{Q}\cdot\mathbf{V}t]\dot G(0,t-t')\sin[\mathbf{Q}\cdot\mathbf{R}_\alpha+\phi(\mathbf{R}_\alpha,t')+\mathbf{Q}\cdot\mathbf{V}t']\ , \tag{27}$$

where $G(\mathbf{R}_\alpha-\mathbf{R}_p,t-t')$ is the Green's function of the system in the absence of the sinusoidal potential and $\dot G$ is its time derivative. Substituting for the sine term from Eq. (25), replacing f using its time Fourier transform, and doing the integrals over t and t' we obtain

$$\mathbf{F}\cdot\mathbf{V}=\frac{1}{TN}c\,|v(Q)|^2\sum_\alpha\int d\omega\sum_p|f_p(\mathbf{R}_\alpha,\mathbf{R}_p,\omega)|^2 \times\frac{1}{N}\sum_{\mathbf{k}}\frac{\gamma\omega^2}{\omega_0(\mathbf{k})^4+\gamma^2\omega^2} \tag{28}$$

in the large-T limit, where p is summed over those values of p for which $-T/2\le t_p\le T/2$, and where $f(\mathbf{R},\omega)$ is the time Fourier transform of Eq. (26), N is the number of atoms in the system, and $\omega_0(\mathbf{k})$ is the frequency of the phonon mode polarized along $\mathbf{Q}$. We have assumed in obtaining this equation that $f_p(\mathbf{R}_\alpha,\mathbf{R}_{p'},\omega)f_{p'}(\mathbf{R}_\alpha,\mathbf{R}_p,\omega)$ is negligible unless $p=p'$ (i.e., the domains do not overlap significantly) or one of the f's is constant and the other is varying rapidly. The contribution to Eq. (27) in such a case is zero since a constant f gives no contribution since it does not create excitations. Using the Debye model to do the sum over $\mathbf{k}$, we obtain

$$\mathbf{F}\cdot\mathbf{V}=\frac{1}{TN}c\,|v(Q)|^2 \times\sum_p\sum_\alpha\int d\omega\,|f_p(\mathbf{R}_\alpha,\mathbf{R}_p,\omega)|^2\gamma^{1/2}\omega^{d/2}\ , \tag{29}$$

where d is the dimensionality of the system. A good estimate for the average

$$\langle\omega^{d/2}\rangle=\frac{\int d\omega\,|f_p(\mathbf{R}_\alpha-\mathbf{R}_p,\omega)|^2\omega^{d/2}}{\int_{\omega\neq0}d\omega\,|f_p(\mathbf{R}_\alpha-\mathbf{R}_p,\omega)|^2} \tag{30}$$

is 2π divided by the time it takes for a domain to jump raised to the $d/2$ power. It is expected that near threshold the domain will spend most of its time in a long-lived unstable configuration and then will move relatively rapidly to another such configuration. During this rapid motion, the unstable mode moves essentially freely under the applied field, and hence its velocity scales as F/γ. Therefore, the jump time is proportional to $1/F$. Then $\langle\omega^{d/2}\rangle\sim F^{d/2}$. The sum

$$\sum_\alpha\int|f_p(\mathbf{R}_\alpha,\mathbf{R}_p,\omega)|^2d\omega =\sum_\alpha\int dt\,|f_p(R_\alpha,R_p,t-t_p)|^2 \tag{31}$$

over t for which f_p is not constant or zero is of the order of the product of the number of sites in the pth domain, N_d, and the time it takes for the pth domain to jump, which is $\sim F^{-1}$ in the large-T limit. Then,

$$\mathbf{F}\cdot\mathbf{V}\sim\frac{1}{TN}c\,|v(Q)|^2\gamma^{1/2}N_dN_jF^{d/2-1}\ . \tag{32}$$

Using the fact that the mean center-of-mass velocity V is proportional to

$$\frac{N_J}{T}\frac{N_d}{N}\ , \tag{33}$$

we obtain

$$F\sim c\,|v(Q)|^2\gamma^{1/2}F^{d/2-1}$$

or

$$F\sim c^{2/(4-d)}|v(Q)|^{4/(4-d)}\gamma^{1/(4-d)} \tag{34}$$

for $d<4$ and $F=0$ for $d\ge4$ [although there exists a nonzero solution for $d>4$, it decreases with increasing $v(Q)$, and hence, is discarded as nonphysical], the threshold field found by Fisher, and earlier by Lee and Rice, in the weak-coupling limit had the same c and $v(Q)$ dependence. An earlier paper by this author[18] gave a different result for F, which is now believed to be erroneous.

Fisher has presented an argument for the existence of a nonzero threshold field in greater than four dimensions, where naive scaling theory predicts that it is zero.[5] It is based on the existence of large but improbable regions in which the phases are locked together so as to produce a

great deal of pinning. The arguments presented in this article for the dynamical threshold field, however, will be applicable even when such strongly pinned regions exist. This implies the existence of a dynamical threshold field which is zero but a static threshold field which is nonzero in greater than four dimensions. Furthermore, even in three dimensions, the arguments presented in this paper apply in both the strong and weak pinning regimes and give the same concentration and potential dependence for the dynamical threshold field, whereas the static threshold field estimated by Lee and Rice[7] has a different dependence in the strong-coupling regime. Then, for sufficiently low impurity concentrations, the dynamical threshold field could be smaller than the static threshold, implying the existence of hysteresis effects like those observed in experiment. In the weak-coupling regime, in fewer than four dimensions, since both static and dynamical threshold fields have the same dependence on potential strength and concentration, it is not possible to determine from the present treatment whether there exists hysteresis in this regime.

V. CONCLUSIONS

We conclude that at least in greater than two dimensions, charge-density-wave motion just above threshold must occur by nonadiabatic motion in which localized domains throughout the system are continually becoming unstable and jumping to new configurations. It is argued that if the motion occurred adiabatically, the dynamical threshold field (i.e., the field below which all motion ceases) would have to be zero. A model based on the above localized domain picture is studied. On the basis of this model, a dynamical threshold field equal to the Lee-Rice field for the weak coupling is found.

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[1]H. Fröhlich, Proc. R. Soc. London, Ser. A **223**, 296 (1954); D. Allender, J. W. Bray, and J. Bardeen, Phys. Rev. B **9**, 119 (1974).
[2]N. P. Ong, Can. J. Phys. **60**, 757 (1982).
[3]G. Gruner, A. Zawadowski, and P. M. Chaikin, Phys. Rev. Lett. **46**, 511 (1981).
[4]R. A. Klemm and J. R. Shrieffer, Phys. Rev. Lett. **51**, 47 (1983).
[5]D. S. Fisher, Phys. Rev. Lett. **50**, 1486 (1983); D. S. Fisher, Phys. Rev. B **31**, 1396 (1985).
[6]H. Fukuyama and P. A. Lee, Phys. Rev. B **17**, 535 (1978).
[7]P. A. Lee and T. M. Rice, Phys. Rev. B **19**, 3970 (1979).
[8]L. Sneddon, M. C. Cross, and D. S. Fisher, Phys. Rev. Lett. **49**, 292 (1982).
[9]J. B. Sokoloff, Phys. Rev. B **23**, 1992 (1981); J. Phys. (Paris) Colloq. **44**, C3-1667 (1983).
[10]J. B. Sokoloff, Phys. Rev. B **16**, 3367 (1977).
[11]J. Bardeen, Phys. Rev. Lett. **42**, 1448 (1979); *ibid.* **45**, 1978 (1980).
[12]L. Pietronero and S. Strassler, Phys. Rev. B **28**, 5863 (1983); N. Teranishi and R. Kubo, J. Phys. Soc. Jpn. **47**, 720 (1979).
[13]G. Grüner, L. C. Tippie, J. Sanny, W. G. Clark, and N. P. Ong, Phys. Rev. Lett. **45**, 935 (1980).
[14]N. P. Ong and K. Maki, Phys. Rev. Lett. **52**, 663 (1984).
[15]P. A. Lee, T. M. Rice, and P. W. Anderson, Solid State Commun. **14**, 703 (1974).
[16]S. N. Coppersmith, Phys. Rev. B **30**, 410 (1984).
[17]J. E. Sacco, J. B. Sokoloff, and A. Widom, Phys. Rev. B **20**, 5071 (1979).
[18]J. B. Sokoloff, in Proceedings of Conference on Low Dimensional Materials in Abara Terme, 1984, edited by J. B. Sokoloff [J. Phys. C (to be published)]; J. Phys. C (to be published).
[19]L. Sneddon, Phys. Rev. Lett. **52**, 65 (1984).
[20]M. Peyrard and S. Aubry, J. Phys. C **16**, 1593 (1983).