Sliding Dynamics of the Incommensurate Chain

Leigh Sneddon
Martin Fisher School of Physics, Brandeis University, Waltham, Massachusetts 02254
(Received 8 July 1983)

The dc dynamics of the sliding incommensurate chain is reduced to a purely static problem. The sliding system is described by a static hull function which becomes singular, above the critical pinning strength, as the velocity approaches zero. Both ac and dc sliding dynamics are determined numerically for the cases of weak and strong pinning and short- and long-range interactions. Excellent agreement is obtained with experiments on sliding charge-density waves near threshold, both in $NbSe_3$ and in TaS_3.

PACS numbers: 72.15.Nj, 72.15.Eb, 72.20.Ht

Incommensurate structures, such as charge-density waves (CDW's) and adsorbed monolayers, are now familiar in solid-state physics.[1] The discovery[2] of electrical conduction due to sliding CDW's raised a wide range of questions concerning the dynamics of sliding incommensurate structures. This article reports progress in the analytic study of such dynamics and in the understanding of related experimental results.

The incommensurate system studied here is a simple extension of the model of Frenkel and Kontorova,[3] and the dimensionless equations of motion can be written

$$\dot{u}_j + \sum_p K_p (2u_j - u_{j-p} - u_{j+p}) = f + P\cos H(j+u_j), \tag{1}$$

where $j = 1, 2, \ldots, N$, P is the strength of the pinning force, and $2\pi/H$ its wavelength. The case of $N\to\infty$ and $H/2\pi$ equal to an irrational, ρ, was studied by considering $H/2\pi = M_N/N$, where M_N is an integer, having no common factor with N, and $M_N/N \to \rho$ as $N\to\infty$.

Equation (1) was Fourier transformed to replace the u_j's by phase-shifted Fourier components $w_m = a_m \exp(i\alpha_m)$:

$$w_m = \exp(-imHw_0)N^{-1}\sum_{j=1}^{N}\exp(-imHj)u_j \tag{2}$$

for $m = 0, 1, 2, \ldots, N-1$. Using Bessel functions to expand the cosine in (1) gives terms with an explicit N dependence. As $N\to\infty$ for a bulk velocity $v > 0$, these terms can be shown to vanish to every finite order of perturbation in P and oscillate at arbitrarily high frequencies about zero. To treat the limit $N\to\infty$, only those terms with no explicit N dependence were retained. This gives

$$v = f + PF_0\{w_m\}, \tag{3a}$$

$$\dot{w}_\mu = -(2[1-\sum_p K_p \cos\mu H_p] + i\mu Hv)w_\mu + PF_\mu\{w_m\} \tag{3b}$$

for $1 \le \mu < N/2$, where

$$F_\mu\{w_m\} \equiv N^{-1}\sum_{j=1}^{N} e^{-i\mu Hj}\cos H[j + 2\sum_{1\le m<N/2} a_m\cos(mHj+\alpha_m)], \tag{3c}$$

independent of w_0.

For constant v, static solutions, with $\dot{w}_\mu = 0$ for $\mu \ge 1$, were found. A finite number, μ_{max}, of the w_μ were retained and the corresponding coupled equations (3b) were solved numerically, treating the retained w_μ to all orders. The couplings in (3c) were computed with N large enough that increasing it had no significant effect. These solutions were tested in two ways. Firstly, the dc characteristic was calculated. With weak pinning, clear convergence, with increasing μ_{max}, to a linear response at $f = 0$ was found, with no threshold. For strong pinning the emergence of a threshold singularity, with increasing μ_{max}, was clearly indicated. The results thus agree with present knowledge[4] at low velocities and are also correct to all orders in perturbation theory at moderate and high velocities. Secondly, the solutions were tested for stability to small perturbations and were found to be dynamically stable.

Since these solutions are static, exploiting translational invariance has transformed the dc sliding dynamics of the infinite incommensurate chain to a purely static problem.

From (2), the Fourier components, y_m, of the distortions then have a simple time dependence:

$y_m = \text{const} \times e^{imHvt}$. (A corresponding result for excitations about the $v=0$ limit was obtained by Novaco.[5]) Further, there is a static hull function describing dc sliding solutions with $v>0$. That is, $u_j - vt$ is a function of a single variable:

$$u_j - vt = g_v(j+vt), \tag{4}$$

where the periodic function g_v is given by

$$g_v(x) = 2 \sum_{1\le m<N/2} a_m \cos(mHx + \alpha_m). \tag{5}$$

Much attention has been given[4,6] to the way, at $f=v=0$, g_v changes from being analytic, for weak pinning, to singular, for strong pinning. The present studies showed the amplitudes a_m decaying exponentially with m when $v>0$, even with strong pinning. The function g_v is then analytic for $v>0$. Thus for strong pinning a breaking-of-analyticity transition occurs in the new hull function, as the velocity approaches zero at threshold. The complicated time dependence of the $u_j(t)$ near threshold is expressed, by (4), completely in terms of the emergence of singularities in this new hull function.

Linear ac response, in the presence of a dc field, has been studied experimentally[7] in the CDW systems $NbSe_3$ and TaS_3. At fields a few times threshold low-order perturbation theory[8] is not useful; but this region is the most commonly studied experimentally because the nonlinear effects are larger than in the high-field region, and sample heating is not a problem. The present techniques were therefore used to determine the ac response of the sliding incommensurate chain near threshold. Having reduced the dc dynamics to a static problem is very useful. The ac response of a time-dependent solution is much more difficult to obtain than that of a static solution, for which the ac response, like the dc characteristics, can be determined without numerical integration.

The CDW's in $NbSe_3$ and TaS_3 are three-dimensionally coherent.[9] One effect of higher dimensionality is to increase the coordination of the system. To mimic this increased coordination crudely, a sixfold-coordinated chain was considered with $K_1 = K_2 = K_3 = \frac{1}{3}$; $K_p = 0$, $p>3$.

By considering in (3) a small perturbation about a static dc solution, the ac response, $\sigma(\omega) = \sigma' + i\sigma''$ was determined, for[10] $p = (5^{1/2}+1)/2$ and $HP = 3.0$. The results (with $\mu_{max} = 15$) for σ' and the dielectric response $-\sigma''/\omega$ are shown in Fig. 1. The basic features in Figs. 1, 3, and 5 are preserved with increasing μ_{max}. The threshold force was estimated from the dc results.

Figure 2 shows experimental results[7] for $\text{Re}\sigma(\omega)$ and $\epsilon(\omega)$ of the sliding charge-density wave in $NbSe_3$. Figure 1 is seen to account well for the voltage and frequency dependence of both

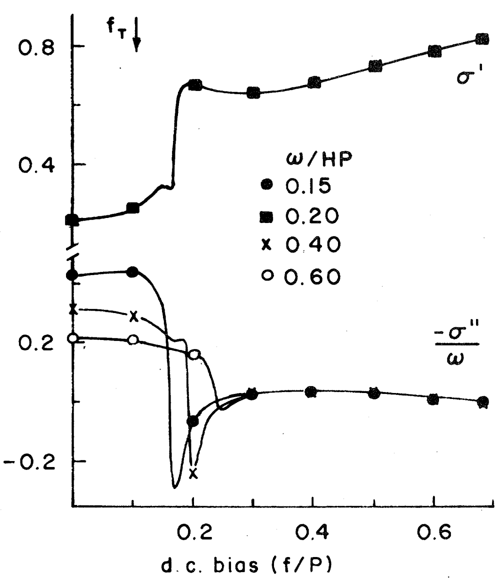

FIG. 1. ac response of sixfold-coordination incommensurate chain, showing interference features.

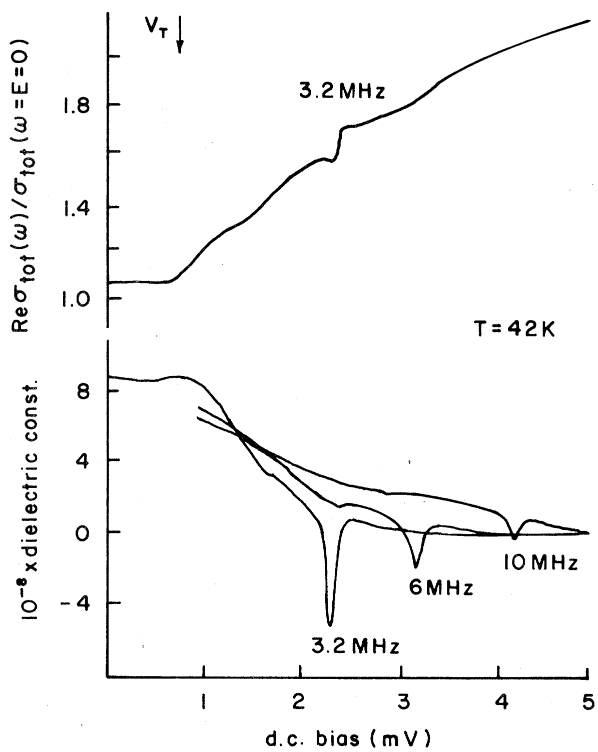

FIG. 2. ac response (Ref. 7) of $NbSe_3$.

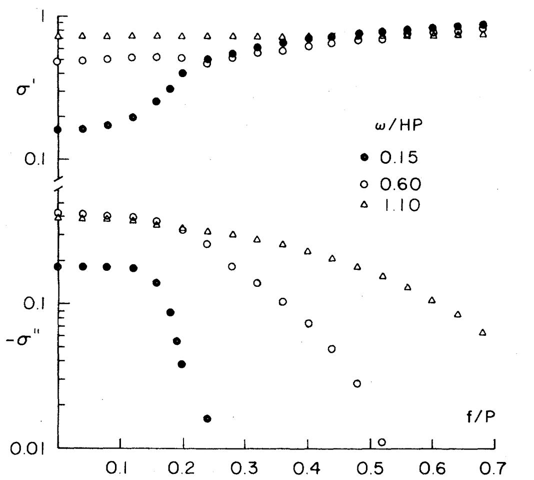

FIG. 3. ac response of incommensurate chain with infinite-range interactions; c.f. Fig. 4 and text.

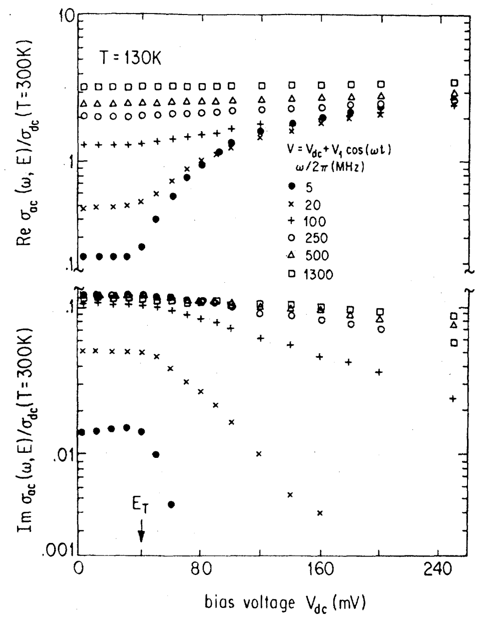

FIG. 4. ac response (Ref. 7) of TaS_3.

components of the ac response. This may not have been expected since CDW dynamics are dominated by randomly positioned defects[11] while the chain is in a periodic potential.

In experiments[7] performed on TaS_3 at 130 K, the sharp interference features seen[7] with $NbSe_3$ (Figs. 1 and 2) were not observed. TaS_3 becomes a semiconductor[12] below the CDW transition, while $NbSe_3$ is metallic.[2] At 130 K the conductivity of TaS_3 has fallen two orders of magnitude from its value at the transition. As discussed earlier,[13] this reduces the screening capacity of the normal electrons and can allow long-range Coulomb interactions of the CDW with itself.

The sliding dynamics of Eq. (1) with long-range interactions, $K_p = 2/N$ for all p, was therefore determined. The results (with $\mu_{max} = 20$) are shown in Fig. 3, and can be compared with the experimental results in Fig. 4. Not only does including long-range interactions account for the absence of interference features, but the properties of the incommensurate chain are seen to match those of TaS_3 extremely well. The *difference* between the ac properties of $NbSe_3$ and TaS_3 can now be understood for the first time as being due to the presence in TaS_3, as suggested earlier,[13] of long-range Coulomb interactions of the CDW with itself.

The ac response was also determined with $f = 0$, and compared to the dc conductivity v/f. The results (with $\mu_{max} = 20$) are shown in Fig. 5 for long-range interactions. Similar results were obtained for the sixfold-coordinated chain. The experimentally observed[14,15] scaling, of field- and frequency-dependent conductivities, is thus exhibited by this *classical* model, and can no longer be regarded[15] as evidence for a quantum mechanical theory of CDW conductivity.

Although these calculations do not probe asymptotic low-frequency threshold properties it is interesting to speculate that the detailed form of the potential becomes less important as one approaches threshold. In any case, the comparison of theory with experiment seen in Figs. 1–5 shows that, in fields comparable to threshold, the incommensurate chain gives a much better picture of CDW dynamics than might have been suspected.

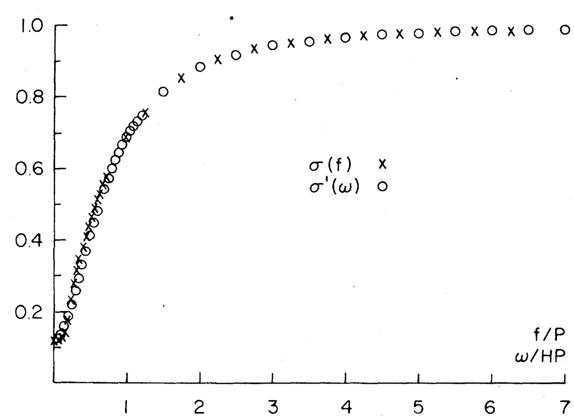

FIG. 5. Scaling of field-dependent (crosses) and frequency-dependent (circles) conductivities in the classical chain.

The author enjoyed discussions with S. Coppersmith, M. Cross, D. Fisher, E. Gross, and P. Littlewood, and thanks A. Zettl and G. Grüner for permission to reproduce experimental results prior to publication.

[1]P. Bak, Rep. Prog. Phys. 45, 587 (1982).

[2]P. Monceau *et al.*, Phys. Rev. Lett. 37, 602 (1976).

[3]Y. I. Frenkel and T. Kontorova, Zh. Eksp. Teor. Fiz. 8, 1340 (1938); F. C. Frank and J. H. van der Merwe, Proc. Roy. Soc. London, Ser. A 198, 205 (1949).

[4]M. Peyrard and S. Aubry, J. Phys. C 16, 1593 (1983).

[5]A. D. Novaco, Phys. Rev. B 22, 1645 (1980).

[6]S. J. Shenker and L. P. Kadanoff, J. Stat. Phys. 27, 631 (1982).

[7]A. Zettl and G. Grüner, to be published.

[8]L. Sneddon, M. C. Cross, and D. S. Fisher, Phys. Rev. Lett. 49, 292 (1982).

[9]R. M. Fleming *et al.*, Phys. Rev. B 18, 5560 (1978); K. Tsutsumi *et al.*, J. Phys. Soc. Jpn. 44, 1735 (1978).

[10]All the results presented here hold for any $H=2\pi p$ (mod2π).

[11]N. P. Ong *et al.*, Phys. Rev. Lett. 42, 811 (1979).

[12]T. Takoshima *et al.*, Solid State Commun. 35, 911 (1980).

[13]L. Sneddon, to be published.

[14]G. Grüner, Mol. Cryst. Liq. Cryst. 81, 17 (1982); A. Zettl *et al.*, Phys. Rev. B 26, 5773 (1982); G. Grüner *et al.*, Phys. Rev. B 24, 7247 (1981).

[15]J. Bardeen, Phys. Rev. Lett. 45, 1978 (1980); A. Zettl and G. Grüner, Phys. Rev. B 25, 2081 (1982); J. Bardeen, Mol. Cryst. Liq. Cryst. 81, 1 (1982); J. H. Miller, Jr., J. Richard, J. R. Tucker, and J. Bardeen, Phys. Rev. Lett. 51, 1592 (1983).