

Oscillatory Instability in the Dynamics of Incommensurate Structures

Leigh Sneddon

Martin Fisher School of Physics, Brandeis University, Waltham, Massachusetts 02254

and

Kenneth A. Cox

Philip Morris Research Center, Richmond, Virginia 23261

(Received 27 March 1985)

We report the discovery of an oscillatory instability in the dynamics of incommensurate structures. The oscillations survive the thermodynamic limit. The instability occurs for both long- and short-range interactions. The frequency and stability of the oscillations are studied.

PACS numbers: 72.70.+m, 72.15.Eb, 72.15.Nj, 72.20.Ht

Quasiperiodic or incommensurate systems have attracted considerable interest in a wide variety of contexts, including adsorbed layers, structures of solids, the onset of chaos, and localization (see, for example, Refs. 1-3). They also exhibit⁴ a variety of the nonlinear properties of sliding charge-density waves (CDW's), including dc characteristics, ac response, ac-dc interference, and electromechanical properties.

We report the discovery of a new phenomenon, a bulk oscillatory instability, in the dynamics of sliding incommensurate structures; and we study some of its properties. The existence of bulk oscillations is surprising since the general belief has been that the phase of any oscillations in a sliding noncommensurate system would vary through the sample, thus cancelling the oscillations in the thermodynamic limit, as indeed occurs in perturbation theory.^{5,6} The instability is therefore breaking the translational symmetry of the bulk noncommensurate system. Finally, in the light of this new result, we discuss the long-standing problem of oscillatory voltage fluctuations in CDW conductors.⁷⁻¹¹

The first model we consider is one for whose dc properties an exact solution is available,⁴ namely, a set of N particles, all interacting equally with each other, subject to a pinning force $P(x)$ and a uniform force F :

$$\dot{U}_j = P(Hj + U_j) + \langle U \rangle - U_j + F. \quad (1)$$

Here H is the lattice spacing; U_j is the displacement of the j th particle (so that $Hj + U_j$ is its position); $\langle U \rangle = N^{-1} \sum_{j=1}^N U_j$; $P(x + 2\pi) = P(x)$; and we study the limit $N \rightarrow \infty$ and $H/2\pi = \text{an irrational}$. Because CDW's are overdamped,^{5,12} purely relaxational dynamics is used. This model can be thought of as a mean-field theory for the incommensurate chain. Following a simple construction¹³ it can be shown, however, that it can also be considered a mean-field theory of a CDW subject to a spatially *random* distribution of identical pinning centers. (With infinite-range interactions, the distinction between the quasiperiodic phase variable Hj and a com-

pletely random phase variable β_j is irrelevant.) It has also provided⁴ accounts of ac-dc interference experiments in the CDW compound TaS₃, and the scaling of field- and frequency-dependent conductivities.

The exact dc solution of this model is⁴ $U_j(t) = vt + g(Hj + vt)$ where $g(x)$ is the solution of the boundary-value problem

$$v(1 + g') = P(x + g) - g, \quad g(x + 2\pi) = g(x).$$

This solution was used here as the initial configuration for a numerical integration of (1), with N particles, and it was checked that the numerical procedure was stable. By addition of any small perturbation the dynamic stability of this solution can be studied. The voltage (F) versus time plot in Fig. 1 shows the result of such a study. The results presented in Figs. 1 and 2 are¹⁴ for $P(x) = 8 \sin x + 12 \sin 4x$.

It is immediately apparent that the dc solution is dynamically *unstable*, with oscillatory fluctuations growing exponentially at first and then saturating. The ap-

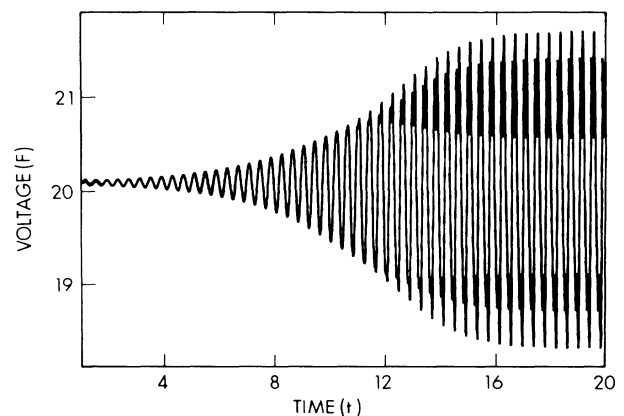


FIG. 1. Voltage vs time for mean-field theory, with $v = 10$. Note the exponential divergence followed by saturation, characteristic of an instability in a nonlinear system.

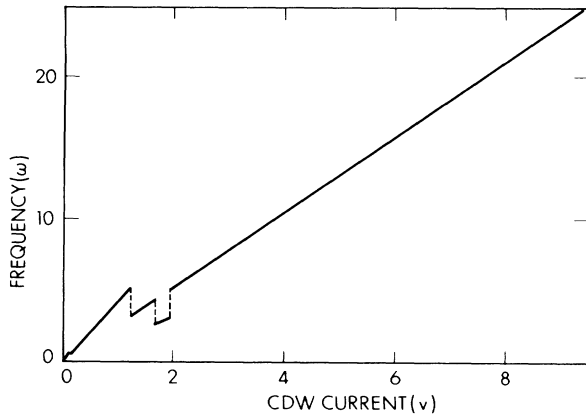


FIG. 2. Frequency vs velocity for the Frenkel-Kontorova model. The segments satisfy $v/\omega = (H/2\pi)^n$ where $n=2$ for the largest segment and cascades through $n=1,2,3,4$ as the velocity is decreased further.

pearance of harmonic content in $F(t)$, as well as saturation, are both due to nonlinearity and they are seen to occur at the same time, as expected. Time series obtained with $N=144, 233$, and 377 are essentially indistinguishable. Thus the results shown in Fig. 1 describe the thermodynamic limit and are not a finite-size effect. Moreover, a finite-size effect would not be expected to show the exponential divergence seen in Fig. 1, which is instead the signature of a dynamic instability.

In addition, we performed a stability analysis of the dc solution to (1) in the limit $N \rightarrow \infty$. CDW experiments are often current driven, and so we considered (1) in the presence of "normal electrons" by keeping fixed a total current, $v + \sigma_n F$, where σ_n is the conductivity of the linear, normal channel. It can be shown that, for *any* pinning potential, oscillations at (complex) frequency ω will occur under conditions of fixed total current $v + \sigma_n F$ only if ω is a root of $\sigma(\omega) = -\sigma_n$ where $\sigma(\omega)$ is the linear response function of the sliding structure. Thus, while an instability under conditions of fixed voltage F would correspond to a pole of σ crossing into the upper-half complex ω plane, the instability shown in Fig. 1, at fixed current v , corresponds to a *zero* of σ crossing into the upper-half plane. We solved the linear-response equation and obtained the zeros of σ for different velocities. At $v=10$ the result was a normal-mode frequency whose real and imaginary parts both agreed precisely with the diverging oscillation seen in Fig. 1, confirming that it shows an oscillatory dynamic instability inherent in the mean-field theory of the dynamics of incommensurate structures.

We calculated the complex normal-mode frequency at different velocities. As the velocity decreases below 11, the zero moves into the upper-half complex plane, signaling an instability of bifurcation. There is thus a critical velocity v_c above which the dc solution is stable (oscillations decay) and below which the oscillations persist.

The instability was observed for a wide range of σ_n , with v_c decreasing as σ_n increases.¹⁵

The solution of the linear fluctuation equation at v_c , $\delta U_j t = \eta(Hj + vt)e^{-i\omega t}$, provides some rudimentary insight into the origin of the instability. The exact solution of the dc motion⁴ showed that there are values of the pinning potential (essentially the peak values) which a locally stable static solution avoids by having discontinuities in the function $g(x)$ defined above. Static solutions do exist with particles in these regions, but such solutions are unstable.⁴ A sliding system, however, must have particles in these regions and a continuous $g(x)$, with dg/dx sharply peaked in these regions for small v . We find that the unstable fluctuation $\eta(x)$ has $|\eta|$ largest just where dg/dx is peaked. Thus the oscillatory instability of the dc solution may be in some measure a dynamic consequence of the existence of unstable static states.

To see whether the oscillatory instability exists in finitely coordinated systems we studied a minimally coordinated system: an incommensurate chain with only nearest-neighbor interactions,¹

$$\dot{U}_j = P(H_j + U_j) + U_{j-1} - 2U_j + U_{j+1} + F. \quad (2)$$

The incommensurate chain has been shown⁴ to give an account of the difference between the ac and dc interference properties of NbSe₃ and TaS₃. A previously obtained⁴ dc solution to (2) was used as an initial configuration in a numerical integration with N particles. Increasing N sufficiently produced identical plots, ensuring that the results represented the thermodynamic limit. Different pinning potentials were studied. So long as $P(x)$ produced a threshold, whether or not $P(x)$ contained harmonics, resulting voltage-time plots showed precisely the exponential instability, followed by saturation, that was seen in Fig. 1 for the mean-field case.

Thus the instability occurs at coordination number infinity and two. It is therefore expected to occur in incommensurately pinned systems at all intermediate coordinations in one, two, and three dimensions.

The oscillation frequency as a function of v , for nearest-neighbor interactions and the same $P(x)$ as in Fig. 1, is shown in Fig. 2 and has some interesting features. It is predominantly linear. Further, although the large- v limit has transients with the trivial frequency $\omega = v$ which would be exhibited by a single particle in $P(x)$, once the instability takes over ($v \leq 9$) a new characteristic frequency and length appear which are determined not only by $P(x)$, but also by the sliding structure itself. In the large linear region in Fig. 2, $v/\omega = (H/2\pi)^2$. That is, the oscillatory instability reveals the length scale H provided by the lattice spacing, which is the length scale corresponding to the wavelength of a CDW.

Further, as v is decreased, there are a number of first-order transitions, where v/ω changes abruptly, being

given by $(H/2\pi)^n$, $n=2,1,2,3,\dots$ as the velocity is decreased.

The properties of the Frenkel-Kontorova model [Eq. (2)] have attracted a great deal of attention (see, e.g., Ref. 2). It is now clear that its dynamic properties are considerably richer than previously realized.

Turning to CDW conductors, the dominant source of pinning is believed to be a random potential due to lattice defects. While Eq. (1) is also a mean-field theory of random pinning, we do not yet know whether a bulk oscillatory instability also occurs in systems with random pinning and short-range interactions.

No critical velocity, v_c , has been reported in the experimental literature. Some experiments in the time domain have, however, revealed transient oscillations.¹⁶ While the existence of transients has no clear explanation within the finite-size^{13,17} or contact¹⁸ theories, a natural interpretation in the present context is that in these experiments $v > v_c$ so that fluctuations oscillate but decay.

The origin of CDW voltage oscillations remains an open question. The unexpected observation of bulk oscillations in models which have exhibited a wide variety of other properties of sliding CDW's may be the basis for the answer, or merely a tantalizing coincidence.

In conclusion, we have reported the discovery of new phenomenon—an oscillatory instability—in the dynamics of incommensurate structures.

We wish to thank P. W. Anderson, E. P. Gross, A. J. Kassman, A. C. Lilly, R. J. Maher, P. Monceau, and A. D. Zima for stimulating discussions. One of us (L.S.) is grateful to Philip Morris, Inc., for the hospitality of the Philip Morris Visiting Scientist Program, and to the Air Force Office of Scientific Research for support under Grant No. 84-0014.

¹Y. I. Frenkel and T. Kontorova, *Zh. Eksp. Teor. Fiz.* **18**, 1340 (1938); F. C. Franck and J. H. van der Merwe, *Proc. Roy. Soc. London, Ser. A* **198**, 205 (1949).

²P. Bak, *Rep. Prog. Phys.* **45**, 587 (1982), and references therein, and *Phys. Rev. B* **32**, 5764 (1985); S. J. Shenker and L. P. Kadanoff, *J. Stat. Phys.* **27**, 631 (1982); M. Peyrard and S. Aubry, *J. Phys. C* **16**, 1593 (1983).

³J. M. Greene, *J. Math. Phys.* **20**, 1183 (1979); L. P. Kadanoff, *Phys. Rev. Lett.* **47**, 1641 (1981); M. J. Feigenbaum, L. P. Kadanoff, and S. J. Shenker, *Physica (Amsterdam)* **5D**,

370 (1982); S. J. Shenker, *Physica (Amsterdam)* **5D**, 405 (1982); T. Ishi, *J. Phys. Soc. Jpn.* **52**, 168 (1983); M. Kohmoto, L. P. Kadanoff, and Chao Tang, *Phys. Rev. Lett.* **50**, 870 (1983); S. Ostlund, R. Pandit, D. Rand, H. Schellnhuber, and E. Siggia, *Phys. Rev. Lett.* **50**, 1873 (1983); R. MacKay, Ph.D. thesis, Princeton University, 1982 (unpublished); T. Janssen, in *Incommensurate Phases in Dielectrics*, edited by R. Blinc and A. Levanyuk (North-Holland, Amsterdam, 1986).

⁴L. Sneddon, *Phys. Rev. Lett.* **52**, 65 (1984), and *Phys. Rev. B* **30**, 2974 (1984), and *Phys. Rev. Lett.* **56**, 1194 (1986).

⁵L. Sneddon, M. Cross, and D. S. Fisher, *Phys. Rev. Lett.* **49**, 292 (1982).

⁶The leading order result of Ref. 5 holds to all orders: see L. Sneddon, *Phys. Rev. B* **29**, 725 (1984).

⁷R. M. Fleming and C. C. Grimes, *Phys. Rev. Lett.* **42**, 1423 (1979).

⁸P. Monceau, J. Richard, and M. Renard, *Phys. Rev. Lett.* **45**, 43 (1980), and *Phys. Rev. B* **25**, 948 (1982).

⁹G. Grüner *et al.*, *Phys. Rev. B* **23**, 6813 (1981).

¹⁰P. Monceau *et al.*, *Phys. Rev. B* **28**, 1646 (1983), and references therein.

¹¹See Proceedings of International Symposium on Nonlinear Transport and Related Phenomena in Inorganic and Quasi One-Dimensional Conductors, Hokkaido University, Sapporo, Japan, 1983, edited by Y. Abe *et al.* (to be published), and *Proceedings of the International Conference on Charge Density Waves in Solids, Budapest, 1984*, edited by Gy. Hutiray and J. Sólyom, *Lecture Notes in Physics* Vol. 217 (Springer-Verlag, New York, 1985).

¹²G. Grüner, L. C. Tippie, J. Sanny, W. G. Clarke, and N. P. Ong, *Phys. Rev. Lett.* **45**, 935 (1980).

¹³D. S. Fisher, *Phys. Rev. Lett.* **50**, 1486 (1983), and *Phys. Rev. B* **31**, 1396 (1985).

¹⁴Harmonic content in $P(x)$ was necessary for the instability to occur with infinite-range interactions but not with finite-range interactions. In all cases we used periodic boundary conditions with $N=N_i$, $H/2\pi=N_{i-1}/N_i-(\sqrt{5}-1)/2$ as $i \rightarrow \infty$.

¹⁵A v_c which vanishes in the fixed-force limit ($\sigma_n \rightarrow \infty$) would explain why studies which were done in this limit did not detect the instability [Ref. 13 and S. N. Coppersmith, *Phys. Rev. B* **30**, 410 (1984)]. In a fixed-voltage or fixed-current experiment the local electric field fluctuates. Whenever, by choosing α_n finite, we allowed f to fluctuate, the dc solution near threshold was unstable and oscillations persisted.

¹⁶M. Oda and M. Ido, *Solid State Commun.* **50**, 879 (1984); R. M. Fleming, L. F. Schneemeyer, and R. J. Cava, *Phys. Rev. B* **31**, 1181 (1985).

¹⁷R. A. Klemm and J. R. Schrieffer, *Phys. Rev. Lett.* **51**, 47 (1983).

¹⁸N. P. Ong, G. Verma, and K. Maki, *Phys. Rev. Lett.* **52**, 663 (1984).