The dc dynamics of models of incommensurate charge density wave (CDW) conductivity was reduced to a purely static problem. The dc characteristics of the incommensurate chain have been determined. A microscopic understanding of differences in nonlinear electrical properties of different CDW materials has been obtained. The experimentally observed scaling of field- and frequency-dependent conductivities was shown to occur in classical systems and can therefore no longer be regarded as evidence of quantum tunneling. The dynamic threshold of incommensurate charge density wave conductivity was seen to be described by a new characteristic function, in which singularities emerge as the velocity approaches zero. The dynamics of the incommensurate chain with long range interactions has been solved exactly, using both analytic and graphical techniques. This complete solution provides direct insight into nonlinear sliding conductivity.
Theory of Sliding Charge Density Waves

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I. Summary of Progress

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II. Research Objectives

The goal of the proposed research is to answer specific major theoretical questions concerning charge density wave (CDW) conductivity, and the dynamics of related lattic systems.

The specific objectives are as follows

II. 1. Voltage Oscillations

CDW conductors generate an ac voltage signal in addition to the dc voltage, when driven with a purely dc current. The origin of these oscillations remains uncertain. One possibility which has been suggested by the PI is that, as in many nonlinear systems, there may be more than one solution to the equations of motion. It may be that the purely d.c. solution, obtained using perturbation theory, is dynamically unstable, and that a dynamically stable, oscillatory solution also exists and is the physical, experimentally observed solution.
The objective of this project is to study the dynamic stability of the dc solution to determine whether it is indeed unstable to an oscillatory motion.

The origin of the voltage oscillations is one of the major outstanding puzzles in CDW dynamics.

II. 2. Long Range Forces

a) Coulomb interactions in TaS$_3$ and NbS$_3$.

Normal electron flow screens the charge accumulations due to CDW distortions. This screening can result in enhanced dissipation, particularly when the normal conductivity decreases from its value at the CDW transition by several orders of magnitude, as in the cases of TaS$_3$ and NbS$_3$. This effect has been dealt with in Publication Number 2.

At even lower normal conductivities, CDW-CDW Coulomb interactions become important. The long wavelength response of the CDW changes in character from being phonon-(or "phason-") like to being plasmon-like. The observation of a drop in the normal conductivity of TaS$_3$ and NbS$_3$, of up to six or seven orders of magnitude, indicates that Coulomb interactions may be important for CDW dynamics at low temperatures in those compounds.

It is therefore proposed to study the effect of Coulomb interactions on CDW transport in the high field region.

b) Infinite Range Forces

For electric fields $E$ near threshold, the current $I$ of a CDW with infinite range interactions, interacting with random defects obeys $I_{\text{CDW}} \sim (E - E_T)^{3/2}$. This concave-up I-V relation contrasts sharply with the concave-down results for the short range, incommensurate chain. It is proposed to study the infinite range, incommensurate case and see whether it behaves like the infinite range, random defect system.
It is also proposed to use the k-space method of Publication 4 to study Coulomb interactions in one dimension and compare the I-V properties with those of systems with short range interactions and those of systems with infinite range interactions.

These studies will provide a reasonably complete picture of the effect of the range of interactions on CDW dynamics.

II. 3. A.C. Response

a) "Scaling"

It is found experimentally that, by suitably scaling either the frequency or field axis, plots of the Ohmic $\sigma(\omega)$ and the nonlinear $\sigma(E) \equiv j_{\text{CDW}}/E$ can be superposed to a good accuracy for $E \gtrsim 3E_T$. Further, it is often claimed that this "scaling" provides major support for the quantum mechanical theory of sliding CDW's.

Preliminary results indicate that the "scaling" which is seen experimentally is also seen in the properties of classical models. It is proposed to investigate to what extent the classical incommensurate chain exhibits this "scaling." The results of this work could play a major role in clarifying the uncertainty which exists in the literature, over whether a classical or a quantum description is required to understand the bulk dynamics of a sliding CDW.

b) The dielectric constant

The dielectric constant $\varepsilon_{\omega}(\omega) \equiv 1 - (\varepsilon_0)^{-1} \text{Im}\sigma(\omega)$, in different d.c. fields $E$ near threshold, has been measured. It is straightforward to see that the results cannot be accounted for by any single particle model.

It is therefore proposed to determine $\varepsilon(\omega)$ for the incommensurate chain with both short and long range interactions, to see if the inclusion of internal degrees of freedom accounts for the experimentally observed behavior.
This will provide a new test of the classical picture of CDW dynamics.

c) Nonlinear time-dependent response

Pronounced metastable and hysteresis effects have been observed experimentally at low CDW velocities. There is as yet no theory of this behavior and it is proposed to see whether the incommensurate chain exhibits these phenomena.

II. 4. Threshold Dynamics

When $E + E_T$ in the incommensurate chain, the chain becomes strongly distorted at all length scales. This indicates that a satisfactory theory of threshold dynamics must include distortions or fluctuations at arbitrarily long length scales. This is clearly reminiscent of equilibrium critical phenomena, an adequate theoretical treatment of which is given only by the renormalization group of Kadanoff, Wilson and Fisher. Threshold dynamics may represent the deepest theoretical challenge in CDW transport. This project, the most difficult in the proposal, is to construct a renormalization group theory of threshold dynamics, starting with incommensurate systems and guided by the theory of equilibrium critical phenomena.

II. 5. Harmonic Mixing and Rectification

CDW's have been seen experimentally to exhibit harmonic mixing and rectification of ac signals. No clear, satisfactory theory of these phenomena exists. It is proposed therefore to model these phenomena in incommensurate structures.

II. 6. Mechanical - Electrical Coupling

In some fascinating recent experiments, the onset of nonlinear CDW conductivity has been observed to produce strong changes in the mechanical properties of CDW systems. It is proposed to study this new phenomenon by treating the coupling to mechanical degrees of freedom in the host lattice.
II. 7. **Polymer Liquid Crystals**

The extreme length of the polymer molecules in polymer liquid crystals leads to a variety of interesting mechanical properties, as well as strong couplings between mechanical and electromagnetic responses. These in turn lead to striking macroscopic phenomena such as instabilities, complex textures and field induced structural changes.

The study of the special effects of extreme molecular length in polymer liquid crystals is still reasonably young. It is proposed to begin by studying elastic constants, in particular to clear up the uncertainty as to how the splay elastic constant depends on molecular length.

This project is stimulated by the opportunity to collaborate with an experimentalist in my own department, R. R. Meyer, who is recognized as a leader in the broad, technologically important, area of liquid crystal physics.

III. **Status of Research**

Project II.2 and parts a) and b) of project II.3 have been completed. Projects II.1 and II.6 are in advanced stages. A number of unanticipated advances have occurred.

The following are the principal research results.

III. 1. The translational invariance of incommensurate systems has been exploited to transform the dc dynamics of the incommensurate chain to a purely static problem. This result, although it sounds rather formal, allows many previously impossible investigations to be performed. In particular, the following developments have been made possible by this advance.

III. 2. The dc characteristics of the incommensurate chain, with both short and long range interactions, have been determined without numerical integration, over a wide range of dc fields.
III. 3. The ac response in the presence of a dc current has been determined, allowing a detailed study of ac/dc interference effects.

The presence of sharp interference features in NbSe$_3$ is seen to depend on the screening effects of uncondensed electrons. The qualitatively different behavior of TaS$_3$ was seen, for the first time, to be due to long range Coulomb interactions in the CDW. This is the first time a microscopic understanding of the differences in nonlinear electrical properties of different CDW materials has been obtained.

III. 4. The experimentally observed scaling of field-and frequency-dependent conductivities has been claimed by J. Bardeen and others to support a quantum tunnelling theory of CDW dynamics. This theory has been at the core of a major controversy in the field. The above scaling was shown by the PI to occur in classical incommensurate systems, and can therefore no longer be regarded as evidence of quantum tunnelling. This appears to be a significant step toward resolving the controversy.

III. 5. The dynamic threshold is seen to be described by a new characteristic function, in which singularities emerge as the velocity approaches zero.

III. 6. The dynamics of the incommensurate chain with long range interactions has been solved exactly, using both analytic and graphical techniques. The ground states and all metastable states are identified. The ac response has a low-frequency singularity at threshold, but the dielectric constant is bounded, as seen in CDW experiments. (Earlier, cruder theories gave a spuriously divergent dielectric response.) The solution was also obtained for the depinning transition; the sliding threshold; and the excitation spectra. This complete steady state solution provides direct insight into nonlinear sliding conductivity and, further, it can now serve as a 'work-horse' for testing new ideas in the field.
III. The PI's proposal that the dc motion of incommensurate structures may be subject to an oscillatory instability has been found to be correct. Information concerning the properties of this instability has been obtained and a manuscript is being prepared.

IV. Publications

6. Oscillatory Instability in the Dynamics of Incommensurate Structures (with K. Cox), in preparation, to be submitted to Physical Review.

V. Interactions and Personnel

The PI has presented the results of this research, by invitation, at the General Meeting of the American Physical Society, Los Angeles, March 1983; and at the International Conference on Charge Density Waves in Solids, Budapest, September 1984.

Dr. K. Cox of the Philip Morris Research Center, Richmond, Virginia has collaborated in some of the research, at no cost to the grant.

VI. Impact

Sliding CDW conductivity constitutes a new form of nonlinear electrical transport. The number of compounds known to exhibit this behavior is at present growing rapidly. This proposal, to solve several major theoretical challenges associated with CDW conductivity, is therefore of significant intrinsic interest in materials research.
Further, the nonlinear aspects of CDW conductivity such as mixing, hysteresis, interference and memory indicate a clear potential for device application.