Fluctuation Conductivity and Lattice Stability in One Dimension*

A. Luther
Department of Physics, Harvard University, Cambridge, Massachusetts 02138

and

I. Peschel
Institut Max von Laue–Paul Langevin, 8046 Garching, Germany
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We calculate the effects of long-wavelength fluctuations on the electrical conductivity and lattice stability of a quasi-one-dimensional metal. Attractive interactions stabilize the lattice and cause a conductivity divergence at zero temperature. These results are exact and can be related to problems in two-dimensional relativistic quantum field theory.

The recent discovery of crystals exhibiting one-dimensional metallic anisotropy,[1,2] has led to renewed interest in the theory and potentialities of such systems.[3-7] The electrical conductivity is of particular interest because of early reports of a giant conductivity[8] in some samples of tetrathiofulvalinium-tetracyanoquinodimethane (TTF-TCNQ). Although attempts to calculate the conductivity for one-dimensional systems have been reported, there are many issues still unresolved.

Neutron-scattering measurements in quasi-one-dimensional magnets, for example $(CD_3)_4NMnCl_3$ (TMMC),[9] have led to considerable insight into the nature of magnetic fluctuations in these systems. As the temperature is raised above the ordering temperature, they exhibit a crossover into a region dominated by one-dimensional spin fluctuations. Part of the interest in quasi-one-dimensional metallic systems arises because of the possibility of useful conductivity enhancement from analogous one-dimensional "superconducting" fluctuations.[3] Three-dimensional ordering need not actually occur, but strong fluctuations must.

We report here the results of a calculation of conductivity enhancement and a study of the related question of lattice stability, based on an exact solution of the Tomonaga or Luttinger model[10] of the interacting one-dimensional electron-lattice system. An exact calculation of the pair susceptibility for this model has exhibited the divergent superconducting fluctuations[11] at zero temperature. The effects of these fluctuations on the impurity or phonon scattering is found to cause significant conductivity enhancement[12] under proper conditions, without necessarily causing a lattice instability. We also remark on the similarity of this fluctuation problem with those encountered in relativistic quantum field theory in two dimensions (one space and time).

We have used a very general microscopic model for the one-dimensional interacting electronic system, including the Fröhlich coupling to the lattice as well as scattering from random impurities. It turns out that processes at the Fermi level are most important, and it is necessary with all of these interactions to distinguish the small-momentum-transfer processes from the large momentum transfer. The former involve scattering near 1 Fermi momentum $\pm k_F$, conserve momentum, and can be solved exactly. The large-transfer processes involve excitations across the Fermi line, with momentum near $2k_F$, cause momentum relaxation, and can be understood in approximate treatments.

The new result which we find for the dc conductivity is given by the formula

$$\sigma = \pi\sigma_0(T)\frac{[\pi k_B T/2W]^g}{2\Gamma(2g)\sin(\pi g)}, \tag{1}$$

where g is related to the screened small-momentum electron-electron interaction V by $g = V\rho \times (1+2V\rho)^{-1}$, and $\Gamma(z)$ is the gamma function. Here ρ is the density of states, $L(2\pi v_F)^{-1}$, W half of the bandwidth, $\sigma_0(T)$ the Born-approximation conductivity for impurity or phonon scattering in the noninteracting electron gas, and we have assumed that $k_B T \ll W\exp(-1/|g|)$. The same result obtains for the small-momentum part of optical-phonon scattering, with the identification $V = -g_s^2/\hbar\omega_0$, where g_s is the electron-phonon coupling constant, ω_0 the phonon frequency, and W replaced by $\hbar\omega_0$. Other excitations, such as excitons, are also described by this formula with obvious identifications. The long-wavelength acoustic-phonon contributions are not important, to the degree that the sound velocity is less than the Fermi velocity.

In deriving this expression for σ, we have assumed the Born approximation for the impurity or phonon scattering at large momentum, and treated the small-momentum part exactly. When $g<0$, from all mechanisms, this is a good approximation because the vanishing scattering rate, given by Eq. (1), indicates that higher-order corrections to the Born approximation are renormalized to zero. Similarly, the large-momentum-transfer part of the electron-electron interaction is reduced for $g<0$, and has therefore been neglected in this formula. For $g>0$, this approximation cannot be defended in general. The conductivity vanishes but corrections are not small, indicating[13] the onset of localization, a topic which we will not consider further here. The divergent conductivity for $g<0$ as $T\to 0$ is consistent with the divergence of the pair susceptibility found previously in that limit.[11] Our results agree with the zero-temperature calculation of the backward-scattering matrix element by Mattis,[13] and with the renormalization-group arguments for weak electron-electron interaction, due to Sólyom.[14]

It is widely believed that low-temperature metallic behavior of one-dimensional systems will be limited by the Peierls lattice instability, converting the metal to a semiconductor. Such an instability would, of course, render the conductivity enhancement of Eq. (1) meaningless. However, an application of our previous calculation shows that a balance between the small- and large-momentum interactions can be found which leads to stabilization of the lattice. The mean-field-theory equation for the Peierls-instability temperature T_P is given by[4]

$$\hbar\Omega = g_L^2\chi(2k_F, T_P), \tag{2}$$

where $\chi(2k_F, T)$ is the static electronic susceptibility at momentum $2k_F$ and temperature T, g_L the electron-phonon coupling constant near $2k_F$, and Ω the phonon frequency in the absence of coupling to electrons. We have solved for $\chi(2k_F, 0)$, treating the small-momentum interactions exactly,[11] and find, for $g<0$,

$$\chi(2k_F, 0) = \rho[-2^{-g}g\Gamma^2(1-g)]^{-1}. \tag{3}$$

Inserting this result into Eq. (2), we determine a critical g_c, such that there is no solution to Eq. (2) for $g<g_c$, and thus no instability. For small g_L, $g_c = \pi g_L^2\rho/\hbar\Omega$, Eq. (3) shows that $\chi(2k_F, 0)$ is a monotone decreasing function of $-g$, so there will always be a solution for g_c. Because fluctuation corrections tend to lower the actual instability temperature,[5] this mean-field estimate is an upper bound on the magnitude of g_c—somewhat weaker attractions are required to fully suppress the Peierls instability.

A small-momentum attraction, $g<g_c$, due to any mechanism, seems to provide the most favorable circumstance to observe conductivity enhancement without lattice instability. Indeed, the one-dimensional model exhibits[11] a "phase transition at $T=0$," which helps to explain the divergent conductivity. For $g>0$, the converse statement is true—the conductivity is decreased, the Peierls transition temperature is increased, and, presumably, problems with localization of the electronic states occur.

It is interesting to consider the experimental data[8,15] on TTF-TCNQ from the viewpoint of Eq. (1). Unfortunately, there are several possibilities and insufficient data at present to determine convincingly the nature of the metal-insulator transition. If a Peierls instability occurs, $g>g_c$, $\sigma_0(T)$ is predominantly caused by phonon scattering at $2k_F$, and the increase in the room-temperature conductivity under pressure[15] can be ascribed to a decrease in g, coupled with an increase in g_L and the bandwidth, which fits the increase in the Peierls temperature. The giant conductivity, reported in some samples,[8] is difficult to understand from Eq. (1), but we believe this equation provides a firm microscopic justification of large fluctuation enhancement.

These results have been derived with the help of the Tomonaga and Luttinger models,[10] which properly describe the small-momentum parts of the problem. The large-momentum processes are studied as perturbative corrections to this model. The Hamiltonian can be written as the sum of two parts, representing this separation, $H = H_s + H_L$, with

$$H_s = H_p + \sum_k v_F k(n_k^{(1)} - n_k^{(2)}) + \tfrac{1}{2}\sum_k V_k \rho_k \rho_{-k} + \sum_k g_s \rho_k \varphi_{-k}, \tag{4}$$

where H_p is the harmonic-lattice Hamiltonian, φ_k a lattice displacement operator, and we have separated the electronic states into those of positive and negative group velocities with $n_k^{(1)}$ and $n_k^{(2)}$ the corresponding number operators. The density operator ρ_k is defined[10] by $\rho_k = \rho_k^{(1)} + \rho_k^{(2)}$, where $\rho_k^{(1)} = \sum_p a_{p+k}^{(1)\dagger} a_p^{(1)}$, etc.; V_k is the electron-electron interaction; g_s the electron-phonon coupling; and

all states up to energy $v_F k_F$ are filled. The label k runs from $-\infty$ to $+\infty$, and it is therefore necessary to introduce a cutoff at the band edges to represent a metal physically. This procedure does not correctly reproduce those features associated with band edges, but does correctly treat excitations near the Fermi level. It is these excitations which lead to infrared singularities, the Peierls instability, and conductivity enhancement; they can be treated exactly. As discussed elsewhere,[10] H_s can be diagonalized because the operators $\rho_k^{(i)}$ satisfy a boson algebra in one dimension, and H_s is therefore bilinear in boson operators.

The large-momentum part of the problem is best expressed in terms of the density operators[11] $\sigma_k = \sum_p a_{k+p}^{(1)\dagger} a_p^{(2)}$, etc., which take electrons from states of one group velocity to the other. In particular, σ_{2k_F} describes excitations across the Fermi line. We write the large-momentum Hamiltonian as

$$H_L = \tfrac{1}{2}\sum_k U_k \sigma_k^{\dagger}\sigma_k + \sum_k g_L \sigma_k \varphi_{-k} + \sum_{k,i} \lambda \sigma_k \exp(-ikR_j) + \text{H.c.}, \tag{5}$$

where U_k is the electron-electron interaction near $2k_F$ and λ represents the effects of scattering from an impurity at site R_j, assumed to be distributed at random. It is seen that $H_L + H_s$ contain the Fermi-surface effects associated with one-dimensional systems, but in a form suitable for application of the exact solution available for H_s.

In order to compute the conductivity result of Eq. (1), we have used a procedure introduced by Götze and Wölfle.[16] Consider, for simplicity, $U_k = g_L = 0$, and write down the equations of motion for the density-density response function, in the basis for which H_s is diagonal. Comparison of this equation with the hydrodynamic equation, which defines the momentum relaxation time, gives the result

$$\tau^{-1} = 2\lambda^2 c(\omega\rho)^{-1} \operatorname{Im}\sum_k \langle\langle \sigma_k ; \sigma_k^{\dagger} \rangle\rangle_{\omega}, \tag{6}$$

where c is the impurity concentration, ω the frequency, and we have used standard notation for the response function.[16] This latter function has been computed exactly,[11] and the result for $\omega \to 0$, Eq. (1), is immediately obtained. Equation (6) exhibits interesting frequency and temperature dependence, which cannot be discussed here because of length restrictions. This result can be readily extended to phonon scattering or, in fact, scattering from any fluctuations.

The response functions appearing in Eq. (2) and Eq. (6), calculated elsewhere,[10] exhibit many similarities (in the zero-temperature limit) with certain vacuum expectation values in the Thirring and Schwinger models of two-dimensional relativistic field theory.[17] These models also have infrared problems, have been solved exactly, and contain essentially the same mathematical problems as the Hamiltonian of Eq. (4). There are trivial differences associated with the band-edge cutoff, and an extra phase factor in the definition of the field operators to account for the Fermi sea. In this older language, the large-momentum part of the interaction described by Eq. (5) corresponds to a scalar coupling of the fields, with scalar coupling to fixed-source fields representing the impurity scattering. The relations between these models have been emphasized by Wightman,[18] but to our knowledge have not as yet been fully exploited in studying the fluctuation problems of interest here. It might be said (with tongue in cheek) that our calculation has determined the temperature dependence of the resistance in the Thirring model.

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Manifestations of Collective Properties of the Degenerate Electron Gas in the $(e, 2e)$ Quasielastic Knockout Process*

V. G. Neudatchin†

Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742

and

F. A. Zhivopistsev

Institute of Nuclear Physics, Moscow State University, Moscow, Union of Soviet Socialist Republics

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It is shown that quasielastic knockout $(e, 2e)$ of electron by a fast electron from a thin solid film presents direct information about both the $\vec{k}$ and ω dependence of the single-particle, spectral-weight function $A(\vec{k},\omega)$ of target electrons. We discuss the expected manifestation of Mahan-Nozières edges and their plasmon satellites in an $(e, 2e)$ experiment side by side with that of plasmaron hole states.

The high-energy, quasielastic knockout of nucleons or nucleon clusters [$(p, 2p)$, (p, pd), etc.] is a powerful tool for nuclear-structure research.[1] Several years ago the $(e, 2e)$ quasielastic knockout process was proposed by Smirnov and one of the authors[2] for the investigation of electron wave functions in atoms, molecules, and thin solid films. Its advantage in comparison with the methods of positron annihilation and Compton scattering profiles[3] consists in the possibility of obtaining the momentum distribution of the target electron for the fixed value of its binding energy side by side with the fixed orientation of its quasimomentum in a monocrystal. The disadvantage of the $(e, 2e)$ method is that it cannot be used for the investigation of thick solid ($d > 250$ Å) or liquid targets.

Subsequent papers have exhibited both various theoretical aspects of the problem mentioned[4-6] (in particular the manifestation of the band structure of solids[2,5,6]) and the first experimental results for solid[7] and gas[8] targets (with the best energy resolution at present[8] $\Delta E \simeq 1-2$ eV). Rather rapid further experimental progress is to be expected.

The first problem considered in the present paper concerns the Mahan-Nozières edges[9] and their plasmon satellites.[10] The main difference between the $(e, 2e)$ process and x-ray absorption considered earlier[9,10] is that the final electron is not near the Fermi surface but is ejected into the high-energy (a few keV) continuum described by plane waves. Thus only the polarization of the degenerate electron gas by the suddenly appearing deep hole is present as a collective effect (high-energy x-ray photoemission would be, of course, similar in this respect). In terms of Ref. 9 we obtain information about singularities of the deep-electron spectral-weight function $Z(\omega)$ itself.

For describing this effect we should generalize the formulas of our previous papers.[2,6] Namely, we should replace the quantity $\delta(\omega - \epsilon_{\vec{p}})\,\delta_{\vec{k}\vec{p}}$ entering into equations for the Sommerfeld model of a degenerate electron gas[2,6] by the general electron spectral-weight function $A(\vec{k}, \omega)$.[11] We obtain

$$\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dE_1 dE_2 d\omega} = \frac{2mk_2}{(2\pi\hbar)^3}\left(\frac{d\sigma}{d\Omega_1}\right)^{\text{free}}_{\text{lab}} NV\delta(E_0 - E_1 - E_2 - \omega)A(\vec{k}, \omega) \qquad (1)$$

as the $(e, 2e)$ cross section for a unit crystal volume containing N electrons (V is the volume of the