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Role of interchain coupling in linear conductors

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Renormalization-group methods are applied to a set of coupled linear chains in a model in which direct hopping between chains is excluded. Attention is focused on models in which intrachain interactions are repulsive. It is shown first for two chains and then for N chains that a repulsive δ-function intrachain interaction scales with decreasing temperature to the attractive fixed point. In the N-chain model this attractive fixed point is characterized by a charge-density wave whose phase is coherent between chains. A variety of response functions, spin and charge density wave at wave vector $2k_F$ (k_F is the Fermi wave vector), and excitonic response functions are calculated numerically. We also evaluate the uniform magnetic susceptibility and the charge-density-wave response at $4k_F$. A comparison is made to the behavior of TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane) at temperatures above 60 K. It is possible to qualitatively explain most of the behavior of this compound by assuming strong repulsion between electrons. A simple physical discussion of the strong-repulsion limit is given.

I. INTRODUCTION

Considerable progress has been made in the theory of one-dimensional metals in the past few years. This theoretical effort has been inspired in part by the discovery of many linear-chain compounds and by the many beautiful experiments on these new materials.[1-4] To date, only limited progress has been made in uniting theory and experiment especially in the organic conductors. Indeed there is as yet no unanimity on whether the interactions are attractive or repulsive in many cases.

There is, however, general agreement among theorists on the properties of a single chain with a nonretarded interaction.[5-10] If the backward-scattering matrix element of the potential is attractive, the system scales to the strong-coupling limit and the charge-density wave and singlet superconductor response functions have power-law divergences at low temperatures. If the backward-scattering matrix element of the potential is repulsive, the interactions scale to the weak-coupling limit and can be described by a combination of renormalization-group and perturbation methods.

In practice one always has interchain coupling. This has been treated in two ways. One approach, which is applicable for attractive intrachain interactions and weak interchain interactions is to solve the single-chain problem first and then treat the interchain interaction within the mean-field approximation.[11,12] When the single-chain correlation lengths become long, this is a very reasonable approach. A second approach has been taken recently by Gor'kov and Dzyaloshinskii[13] who studied the N-coupled-chain problem within the parquet-graph approximation in which interchain and intrachain interactions are treated on the same footing. An alternate method which also treats the interchain and intrachain interactions in the same way is the renormalization-group method and this has been applied to the N-chain problem by Mihaly and Solyom.[14] They calculate the scaling equations for the dimensionless coupling constants up to second order. They show that as the fixed point for attractive intrachain interactions is approached the interchain interactions become long range and that a charge-density wave (CDW), whose phase is coherent in the direction transverse to the chains, is formed at a finite transition temperature.

In this paper we will be concerned with the study of repulsive intrachain interactions. A surprising feature of our results is the demonstration that for δ-function intrachain and interchain interactions the system scales to the attractive strong-coupling fixed point at which there is a phase transition to the CDW phase with long-range order in the transverse directions. The other fixed point of the single chain, characterized by weak interactions, can be reached only from a restricted domain in the space of the bare coupling constants. The boundary between the domains of the two fixed points is not simply determined by the sign of the backward-scattering matrix element but is a more complicated function of the bare coupling constants. For most physically interesting values including the case of a repulsive δ-function interaction of arbitrary strengths on and between the chains, one scales to the attractive fixed point, i.e., CDW phase. Independently Menyhard[15] has shown that interchain coupling can drive a system with repulsive intrachain interaction to the CDW phase. She treated the case of weak interchain coupling and the criterion she obtained is that the single-chain CDW response function diverges.

The outline of the paper is as follows. In Sec. II we start by studying the two-chain problem using the lowest-order renormalization-group equations. We are able to obtain analytically the boundary between the domains of the two types of fixed points in the space of the bare coupling constants. In this section we also consider the N-chain system, but restrict the range of the interaction to nearest neighbors—an approximation which is reasonable near the boundary since the intrachain interaction is repulsive and interchain interaction is short range.

In Sec. III the scaling equations for the N-chain system are Fourier transformed in the transverse direction and solved numerically to obtain the temperature dependence of the dimensionless coupling constants. These are applied in Sec. IV to study the response functions with varying temperature. We apply this method to obtain three classes of response functions: (a) with wave vector $q = 2k_F$ (k_F is the Fermi wave vector), (b) $q = 0$, and (c) $q = 4k_F$. In classes (a) and (b) we study the CDW, SDW (spin-density wave), and Cooper-pair response functions. In addition we study some interchain response functions—in a model with only electron chains they involve Cooper pairs composed of two electrons on neighboring chains and in charge-transfer compounds with electron and hole chains they describe an excitonic response function in which an electron on one chain is correlated with a hole on its neighbor. The characteristic of the intrachain response functions is that over most of the temperature range they resemble the single-chain response functions and it is only at quite low temperatures that the features associated with the attractive fixed point appear. Further, among the $2k_F$ response functions it is only the CDW response that is divergent at the fixed point.

Finally, in Sec. IV we compare our results to experiments on several organic conductors especially TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane). We find that most of the behavior of this compound can be qualitatively explained by the assumptions of strong Coulomb repulsion between electrons.

II. TWO CHAINS

We begin our discussion of the coupled-chain problem by first examining the simpler problem of two chains. The model consists of two linear chains which are strictly one dimensional. There is an interchain potential coupling but interchain hopping is excluded. Each electron can be labeled by an index i which denotes the chain number. The properties of a one-dimensional metal are dominated by the electrons near the Fermi surface. We denote by $\alpha_k^\dagger$ and $\beta_k^\dagger$ the electron creation operators for electrons near $+k_F$ and $-k_F$, respectively, and measure the momenta k from these values. The Hamiltonian for an arbitrary number of chains has the form

$$H = H_0 + H_1 \;, \tag{2.1}$$

with the kinetic-energy term

$$H_0 = \sum_{\substack{k\sigma \\ i}} v_i k (\alpha_{ik\sigma}^\dagger \alpha_{ik\sigma} - \beta_{ik\sigma}^\dagger \beta_{ik\sigma}) \tag{2.2}$$

and interaction term

$$\begin{aligned} H_1 = \sum_i \sum_{\substack{k_1, k_2, k_3 \\ \sigma, \sigma'}} & (g_{1i} \alpha_{ik_1\sigma}^\dagger \beta_{ik_2\sigma'}^\dagger \alpha_{ik_3\sigma'} \beta_{ik_1+k_2-k_3\sigma} \\ & + g_{2i} \alpha_{ik_1\sigma}^\dagger \beta_{ik_2\sigma'}^\dagger \beta_{ik_3\sigma'} \alpha_{ik_1+k_2-k_3\sigma}) \\ + \sum_{i>j} \sum_{\substack{k_1, k_2, k_3 \\ \sigma, \sigma'}} & (w_{1ij} \alpha_{ik_1\sigma}^\dagger \beta_{jk_2\sigma'}^\dagger \alpha_{jk_3\sigma'} \beta_{ik_1+k_2-k_3\sigma} \\ & + w_{2ij} \alpha_{ik_1\sigma}^\dagger \beta_{jk_2\sigma'}^\dagger \beta_{jk_3\sigma'} \alpha_{ik_1+k_2-k_3\sigma}) . \end{aligned} \tag{2.3}$$

The Fermi velocities v_i can in principle depend on chain index but we will assume throughout this paper that $v_i \equiv v$ and drop the suffix. The intrachain interactions are specified by the coupling constants g with g_{1i} denoting backward scattering and g_{2i} forward scattering, and the corresponding interchain interactions by w_1 and w_2. In Fig. 1 the various terms are represented diagrammatically and a solid (dashed) line denotes an electron propagating with momentum near $+k_F$ ($-k_F$). Note that we have entirely neglected any interchain hopping or any interchain exchange of particles. A discussion of these effects can be found in Ref. 12. Also umklapp processes are excluded from Eq. (2.1).

The study of the one-dimensional Fermi gas is interesting because of the singularities in both the Cooper or particle-particle channel and simultaneously in the zero-sound or particle-hole channel. For the single-chain problem the leading logarithmic correction in an expansion in powers of the coupling constants were summed first by

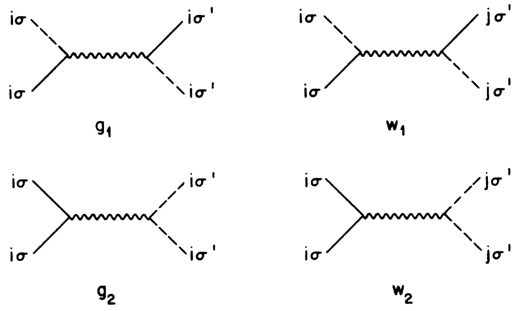

FIG. 1. Basic interactions considered in the model Hamiltonian equation (2.3). Solid (dashed) line denotes an electron propagating with momentum near $+k_F$ $(-k_F)$.

Bychkov, Gor'kov and Dzyaloshinskii[5] using the parquet approximation. Recently Menyhard and Solyom[7] in an elegant paper have applied the renormalization-group method to this problem. In the renormalization-group approach one assumes that a given Hamiltonian with values of the energy cutoff E_F and coupling constants g, w can be transformed into a Hamiltonian with a new cutoff E_F' and new coupling constants g', w'. The one-particle Green's function and the dimensionless vertices are assumed to be multiplicatively renormalizable under the scaling of the cutoff energy. The differential forms of these scaling relationships are the Lie equations of the group. The Lie equations for the coupling constants g, w can be calculated from a perturbation expansion. The leading corrections to the four-point vertex functions are shown in Fig. 2. If the series is truncated at this order, the renormalization-group approach is entirely equivalent to the sum of the parquet graphs.[5]

A system of coupled linear chains has been considered in the parquet approximation by Gor'kov and Dzyaloshinskii[13] and in the renormalization-group method by Mihaly and Solyom.[14] If we specialize their results to two chains which we label as i and j, the Lie equations to lowest order in the coupling constants take the form

$$\begin{aligned}
\frac{\partial g_{1i}}{\partial \xi} &= \frac{1}{2\pi v}(2g_{1i}^2 + 2w_1^2),\\
\frac{\partial w_1}{\partial \xi} &= \frac{1}{2\pi v}[4g_1 w_1 + w_1(2w_2 - g_{2i} - g_{2j})],\\
\frac{\partial g_{2i}}{\partial \xi} &= \frac{g_{1i}^2}{2\pi v},\\
\frac{\partial w_2}{\partial \xi} &= \frac{w_1^2}{2\pi v},
\end{aligned} \tag{2.4}$$

where $\xi = \ln(E_F'/E_F)$. The temperature dependence of the coupling constants can be obtained formally by defining $\xi = \ln(T/E_F)$ and solving Eqs. (2.4).

The four coupled equations (2.4) can be simplified at once by noting that the combinations

$$\frac{\partial \Lambda_i}{\partial \xi} = \frac{\partial}{\partial \xi}\left(\frac{1}{2\pi v}(g_{1i} - 2g_{2i} - 2w_2)\right) = 0, \tag{2.5}$$

and the Λ_i are therefore invariant. Introducing the new variables

$$\begin{aligned}
U_i &= g_{1i}/2\pi v,\\
W &= w_1/2\pi v,\\
V_i &= (1/2\pi v)(g_{1i} - 2g_{2i} + 2w_2),
\end{aligned} \tag{2.6}$$

we can rewrite the set of equations (2.4) as

$$\begin{aligned}
\frac{\partial U_i}{\partial \xi} &= 2U_i^2 + 2W^2,\\
\frac{\partial V_i}{\partial \xi} &= 4W^2,\\
\frac{\partial W}{\partial \xi} &= \tfrac{1}{2}W(3U_i + 3U_j + V_i + V_j).
\end{aligned} \tag{2.7}$$

A. Equivalent chains

Consider first the equivalent chain limit $U_i \equiv U_j$ and $V_i \equiv V_j$. It is clear at once from Eqs. (2.7) that one does not scale away from this limit. There are two fixed points of these equations. One is $U, V \rightarrow -\infty$ and $|W| \rightarrow \infty$ and $U/V \rightarrow 1$ and $|W|/V \rightarrow 1$. The second is $U \rightarrow 0$, $W \rightarrow 0$, and $V \rightarrow$ const. These two fixed points are generalizations of those found for the single chain. The latter is a generalization of the weak-coupling limit obtained in the single-chain problem for $g_1 > 0$. The former is the strong-coupling limit which, of course, is not adequately treated by the first-order renormalization equations. The demarcation between the two regions for a single chain is simply given by the sign of g_1. In the present case this is not the correct criterion as we shall now demonstrate.

The three coupled differential equations (2.7) can be reduced to two by dividing out the ξ variable

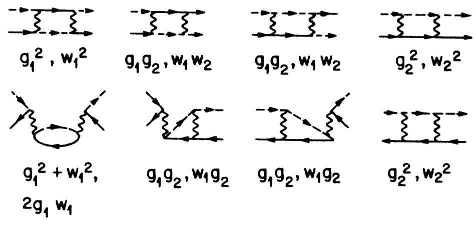

FIG. 2. Corrections to the four-point vertex function which are logarithmically divergent. Coefficients of the intrachain and interchain interactions which enter are shown under each graph.

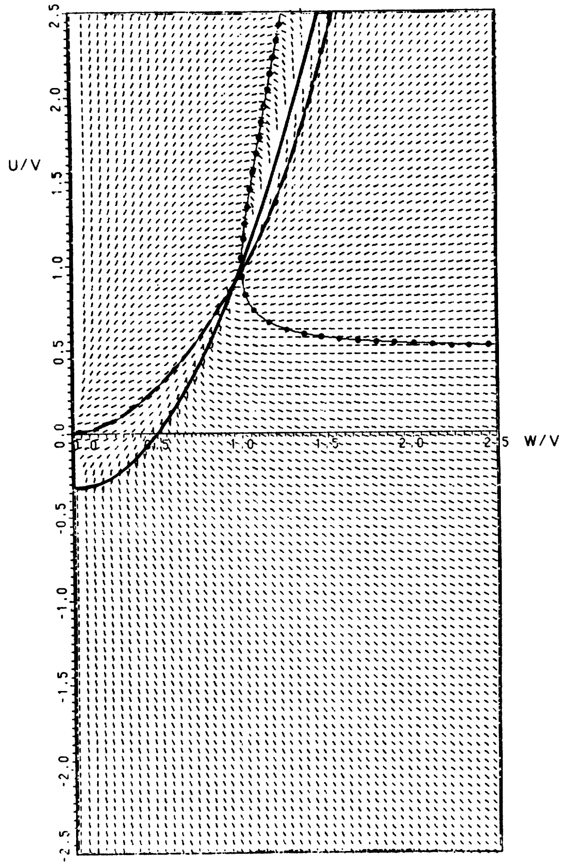

FIG. 3. Slope dx/dy [$=\phi(x,y)$] is plotted at a lattice of points. Dotted and solid lines are those curves at which $\phi=0$ and $\phi=\infty$. Dashed line is the curve $x=y^2$ which is the separatrix of Eq. (2.9).

$$\frac{dU}{dV}=\frac{U^2+W^2}{2W^2}\,,\quad \frac{dW}{dV}=\frac{3U+V}{4W}\,. \tag{2.8}$$

This pair of homogeneous equations can be further simplified by introducing the variables $x(=U/V)$ and $y(=W/V)$. They satisfy the single inhomogeneous equation

$$\frac{dx}{dy}=\frac{2x^2+2y^2-4xy^2}{3xy+y-4y^3}=\phi(x,y). \tag{2.9}$$

The two fixed points given above are at $x=0$ and $y=0$ and $x=1$ and $|y|=1$. We observe at once that by dividing Eq. (2.9) by y it can be written as an equation for y^2. Thus the sign of y is irrevelant. [An examination of Eq. (2.7) shows at once that it can be written as a set of equations involving only W^2.[16]]

At each point in the (x,y) plane the derivative is determined by $\phi(x,y)$. Figure 3 is a plot which shows the derivative at a lattice of (x,y) points. The dotted and solid lines are the loci of points where $\phi(x,y)=0$ and $\phi(x,y)=\infty$. Our aim is to determine the trajectories as ξ varies from 0 (high temperature) to $-\infty$ (zero temperature). These trajectories are determined by drawing continuous curves through the slopes in Fig. 3. At this point it is useful to distinguish between $V>0$ and $V<0$. Clearly if $V<0$, then V will continue to decrease and all trajectories will lead to the fixed point $x=1$, $|y|=1$. For $V>0$, there are two classes of trajectories. One which flows to ∞, or correspondingly $V=0$ and thence unto the $V<0$ plane. The other flows into the origin $x=0$, $|y|=0$. The boundary between the domains of these two fixed points is a curve passing through both. A special solution of Eq. (2.9) which does this is

$$x=y^2. \tag{2.10}$$

This solution is shown as the dashed line in Fig. 3. If we express this solution in terms of the original U, V, W variables, then one gets

$$\frac{\partial}{\partial\xi}(UV-W^2)=2U(UV-W^2). \tag{2.11}$$

Thus $UV=W^2$ is a special solution. Further one cannot cross this solution since the normal derivative goes to zero as one approaches this solution. This special solution forms the boundary also known as the separatrix, between trajectories which scale to the weak-coupling fixed point, U, $W=0$, and $V=$ const and those which scale to the strong-coupling attractive fixed point $U, V\rightarrow-\infty$ and $|W|\rightarrow\infty$. It is possible to solve completely for $U(\xi)$, $V(\xi)$, and $W(\xi)$ along the surface $UV=W^2$ and details are to be found in Appendix A.

The necessary conditions to scale to the weak-coupling fixed point are

$$UV>W^2 \text{ and } U>0;\quad V>0. \tag{2.12}$$

Expressing these conditions in terms of the original coupling constants

$$g_1(g_1-2g_2+2w_2)>w_1^2 \text{ and } g_1>0;\quad g_1-2g_2+2w_2>0. \tag{2.13}$$

If we pass to the limit of δ-function interactions $g_1=g_2=g$ and $w_1=w_2=w$, then these conditions reduce to

$$(g-w)^2<0 \text{ and } g>0;\quad 2w-g>0. \tag{2.14}$$

It follows that for a δ-function interaction the scaling trajectories go to the strong-coupling fixed point irrespective of the sign of the interaction. The novel feature of the two-chain problem is that one can start with a purely *repulsive* interaction and scale to the region of attractive interaction. This feature can be seen explicitly by numerically integrating the starting equations

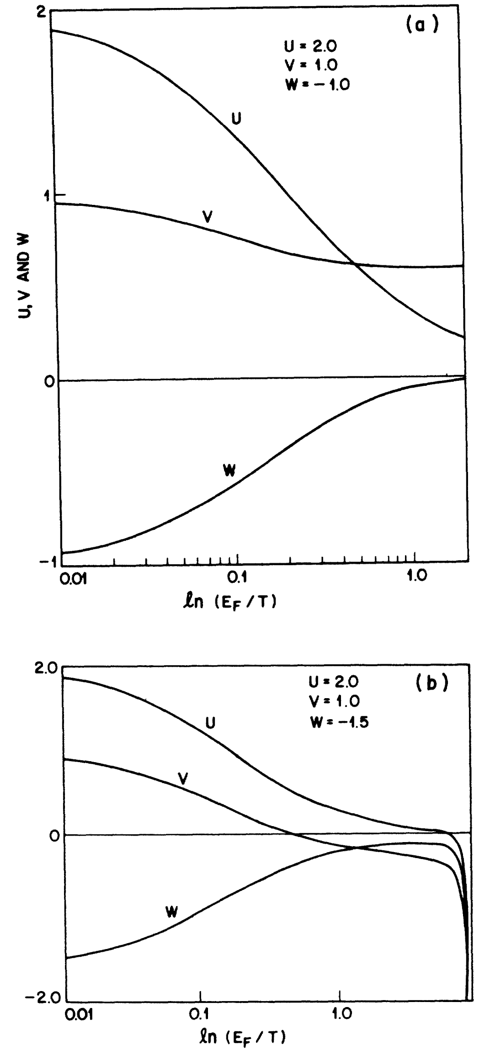

FIG. 4. Two numerical solutions of the coupled set of differential equations which are on opposite sides of the separatrix and scale (a) to the repulsive fixed point and (b) to the attractive fixed point.

(2.7). In Fig. 4 a series of numerical solutions is plotted. The interesting ones are those in which the intrachain g_1 or U starts out repulsive, weakens, and then because of the presence of the w_1^2 in the right-hand side of Eq. (2.4) passes through zero and into the attractive regime. Note that this unusual behavior in which the interaction changes sign occurs at small values of the dimensionless coupling constant—a region where the first-order renormalization equations are most reliable. We shall discuss this further in Sec. III where we demonstrate similar behavior in the N-chain problem.

B. Inequivalent chains

It is of some interest to discuss two inequivalent chains. Starting from Eq. (2.7) it is clear at once that

$$\frac{\partial(V_i - V_j)}{\partial \xi} = 0$$

and (2.15)

$$\frac{\partial(U_i - U_j)}{\partial \xi} = 2(U_i^2 - U_j^2).$$

We see at once that $V_i = V_j + \text{const}$. Introducing the notation

$$U_\pm = \tfrac{1}{2}(U_i \pm U_j); \quad V_+ = \tfrac{1}{2}(V_i + V_j), \tag{2.16}$$

then rewriting we obtain the following set of equations

$$\frac{\partial U_-^2}{\partial \xi} = 8U_-^2 U_+, \quad \frac{\partial U_+}{\partial \xi} = 2U_+^2 + 2U_-^2 + 2W^2,$$
$$\frac{\partial V_+}{\partial \xi} = 4W^2, \quad \frac{\partial W}{\partial \xi} = W(3U_+ + V_+). \tag{2.17}$$

The first equation can be integrated to give

$$\ln\left(\frac{U_-^2}{U_-^2(\xi = 0)}\right) = 8\int_0^\xi U_+(\xi)\, d\xi. \tag{2.18}$$

In the region of attractive values of $U_+(\xi)$ the right-hand side is positive and as the "attractive" fixed point is approached, U_- is also divergent. Therefore at the "attractive" fixed point U_i and U_j do not diverge at the same rate. This suggests we look for a fixed point at which $|U_i| \gg |U_j|, |W|, |V_+|$. Under these conditions U_i obeys an equation

$$\frac{\partial U_i}{\partial \xi} = 2U_i^2, \tag{2.19}$$

which has a solution of the form

$$U_i(\xi) \approx \frac{U_{i0}}{1 - 2\xi U_{i0}}, \tag{2.20}$$

where U_{i0} is a negative constant. The scaling equation for W then reduces to

$$\frac{\partial W}{\partial \xi} = \frac{3U_i W}{2} \tag{2.21}$$

and substituting from Eq. (2.20) we obtain

$$W(\xi) \simeq \frac{W_0}{(1 - 2U_{i0}\xi)^{3/4}}. \tag{2.22}$$

This form may be substituted into Eq. (2.17) to yield

$$V_+(\xi) \simeq 2U_j(\xi) \approx \frac{W_0^2}{U_{i0}} \frac{4}{(1 - 2U_{i0}\xi)^{1/2}}. \tag{2.23}$$

Near the fixed point all of the functions U_i, U_j,

V_+, and W diverge but $|U_i| \gg |W| \gg |U_j|, |V_+|$. At this point we must add the proviso that these results were obtained using first-order renormalization-group equations and are only qualitatively reliable, at best, near the fixed point. In Sec. III the N-chain problem is discussed and their behavior is contrasted to that obtained above.

We turn now to a study of the domains of the three possible fixed points. The boundary between the two attractive fixed points is simply given by the condition $U_i = U_j$. This can be seen at once from the scaling equation for U_- which shows that U_- cannot change sign. We have not succeeded in obtaining the boundary between the repulsive fixed point and the attractive fixed points in closed form as we did for two equivalent chains. We can, however, obtain bounds on the domain of the repulsive fixed points quite simply. First it is clear that a necessary, but not sufficient, condition is that both $U_i > 0$ and $U_j > 0$. [If either U_i or U_j were negative then it is clear from Eq. (2.7) that it would decrease indefinitely.] If both $U_i > 0$ and $U_j > 0$, then we can derive some bounds as follows. First, from Eq. (2.7) one obtains the equations

$$\frac{\partial}{\partial \xi}(U_i V_+ - W^2) = 2U_i(U_i V_+ - W^2) + 3(U_i - U_j)W^2, \tag{2.24}$$

$$\frac{\partial}{\partial \xi}(U_j V_+ - W^2) = 2U_j(U_j V_+ - W^2) - 3(U_i - U_j)W^2. \tag{2.25}$$

If we take $U_j > U_i$ and $U_i V_+ > W^2$, then the second term on the right-hand side of (2.24) is negative and as ξ decreases from zero if the first term becomes small, then the second term will prevent $(U_i V_+ - W^2)$ from changing sign. Thus if both $U_i V_+ > W^2$ and $U_j V_+ > W^2$, then the scaling trajectories lead to the weak coupling repulsive fixed point. One can use a similar argument to prove that if both $U_i V_+ < W^2$ and $U_j V_+ < W^2$, then the scaling trajectories lead to the attractive strong-coupling fixed point.

C. Nearest-neighbor approximation

In Sec. III we will study the N-chain problem in some detail. We can, however, use an approach directly analogous to that given above for the two-chain problem, if we restrict the range of the interchain interaction to nearest neighbor. The nearest-neighbor approximation will break down near the attractive fixed point where Mihaly and Solyom[14] have shown that the range of the effective interchain interaction becomes infinite. However, in determining the boundary between the domain of the repulsive fixed point and the attractive fixed point or points the interactions are short range and it is a reasonable approximation to neglect the next-nearest-neighbor and further interchain interactions.

The first-order renormalization-group equations for an N-chain system in the nearest-neighbor approximation (in this section we consider only N-equivalent chains) are[13,14]

$$\begin{aligned}
\frac{\partial g_1}{\partial \xi} &= \frac{1}{2\pi v}(2g_1^2 + 2zw_1^2),\\
\frac{\partial w_1}{\partial \xi} &= \frac{1}{2\pi v}[4g_1 w_1 + 2z' w_1^2 + 2w_1(w_2 - g_2)],\\
\frac{\partial g_2}{\partial \xi} &= \frac{g_1^2}{2\pi v}, \quad \frac{\partial w_2}{\partial \xi} = \frac{w_1^2}{2\pi v},
\end{aligned} \tag{2.26}$$

where z denotes the number of nearest neighbors and z' is the number of sites which are nearest neighbors to two nearest-neighbor sites (e.g., in a two-dimensional square lattice $z' = 0$, in a two-dimensional triangular lattice $z' = 2$). The combination $\Lambda = (g_1 - 2g_2 - 2zw_2)/2\pi v$ is an invariant. Eliminating Λ we obtain the set of equations

$$\begin{aligned}
\frac{\partial U}{\partial \xi} &= 2U^2 + 2zW^2,\\
\frac{\partial W}{\partial \xi} &= W\left(3U + 2z'W + \frac{(z+1)V + (z-1)\Lambda}{2z}\right),\\
\frac{\partial V}{\partial \xi} &= 4zW^2,
\end{aligned} \tag{2.27}$$

where $V = (g_1 - 2g_2 + 2zw_2)/2\pi v$. For simplicity we consider a planar array of chains, i.e., $z = 2$, $z' = 0$. Then eliminating the ξ variable we get the set of equations

$$\frac{dW}{dV'} = \frac{3U + V'}{6W}; \quad \frac{dU}{dV'} = \frac{U^2 + 2W^2}{3W^2}, \tag{2.28}$$

where $V' = \frac{1}{4}(3V + \Lambda)$. This is also a set of homogeneous equations which can be reduced to a single inhomogeneous equation by transforming to the variables $x = U/V'$ and $y = |W|/V'$

$$\frac{dx}{dy} = \frac{2x^2 + 4y^2 - 6xy^2}{y + 3xy - 6y^3} \equiv \phi_{nn}(x, y). \tag{2.29}$$

The function $\phi_{nn}(x, y)$ has a form similar to the function $\phi(x, y)$ defined in Eq. (2.9) for the two-chain problem. Some of the numerical constants are different. One of the fixed points is at $x = 0$, $y = 0$ as before, but the other has moved to $x = \frac{1}{6}(\sqrt{33} + 3)$ and $y^2 = \frac{1}{12}(\sqrt{33} + 5)$. We can make a plot of $\phi_{nn}(x, y)$ similar to Fig. 3. It has the same general form but it differs in numerical detail. It is straightforward to show that any combination of δ-function interactions, intra- and interchain, lies in the domain of the attractive fixed point.

The conclusion is that the domain of the weak-coupling repulsive fixed point is small and that one can start with purely repulsive interactions and scale to the attractive fixed point. For repulsive interactions there is a strong similarity between the two-chain and N-chain problem.

III. N COUPLED CHAINS

Next we consider the problem of N chains coupled together by electron-electron interaction, again ignoring interchain hopping. The first-order renormalization-group equation has been written down by Gor'kov and Dzyaloshinskii[13]

$$\frac{\partial \gamma_{1ij}}{\partial \xi} = 2\sum_{k} \gamma_{1ik}\gamma_{1kj} + 2\gamma_{1ij}(\gamma_{2ij} - \gamma_{2ii}), \tag{3.1}$$

$$\frac{\partial \gamma_{2ij}}{d\xi} = \gamma_{1ij}^2, \tag{3.2}$$

where

$\gamma_{1ii} = g_{1i}/2\pi v$, $\gamma_{2ii} = g_{2i}/2\pi v$,

$\gamma_{1ij} = w_{1ij}/2\pi v$, $\gamma_{2ij} = w_{2ij}/2\pi v$, and $\xi = \ln(E_F'/E_F)$.

The next-order corrections to these equations have been obtained by Mihaly and Solyom[14] who also studied the fixed-point behavior. They argue that for long-range interaction the first term on the right-hand side of Eq. (3.1) is of order N and will dominate and γ_2 may be neglected compared with γ_1. They show that for attractive interactions one indeed scales from a short-range interaction to a long-range one, and the assumption that $\gamma_2 \ll \gamma_1$ is thus self-consistent. While their analysis approximately describes the behavior near the critical point it does not provide information on the phase boundary in the space of the bare coupling constants. We have seen that for two chains terms analogous to the γ_{2ij} can drive the coupling constant from repulsive to attractive. To investigate similar behavior in the N-chain case it is more convenient to go to Fourier space. Introducing

$$\gamma_1(\vec{q}) = \frac{1}{N} \sum_{ij} e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}\gamma_{1ij} \tag{3.3}$$

and

$$\gamma_2(\vec{q}) = \frac{1}{N} \sum_{ij} e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}\gamma_{2ij}, \tag{3.4}$$

Eqs. (3.1) and (3.2) become

$$\frac{d\gamma_1(\xi,\vec{q})}{d\xi} = 2\gamma_1^2(\vec{q}) + 2\sum_{\vec{q}'} \gamma_2(\vec{q}')[\gamma_1(\vec{q}-\vec{q}') - \gamma_1(\vec{q})], \tag{3.5}$$

$$\frac{d\gamma_2(\xi,\vec{q})}{d\xi} = \sum_{\vec{q}'} \gamma_1(\vec{q}-\vec{q}')\gamma_1(\vec{q}'). \tag{3.6}$$

The qualitative behavior of $\gamma_1(\xi,\vec{q})$ and $\gamma_2(\xi,\vec{q})$ is clear by inspection of these equations. From Eqs. (3.6) or (3.2) it is clear that γ_{2ij} and $\gamma_2(\vec{q}=0)$ decrease monotonically as ξ scales from 0 to $-\infty$ since the right-hand side of the scaling equations are positive. The first term in Eq. (3.5) also tends to decrease γ_1 and by itself would reduce $\gamma_1(\vec{q})$ from a positive value until it is zero. However, the effect of the second term cannot be ignored. In particular, let $\vec{q}_0$ be the $\vec{q}$ value at which $\gamma_1(\vec{q})$ is minimum. Then $[\gamma_1(\vec{q}_0-\vec{q}') - \gamma_1(\vec{q}_0)]$ is positive for all $\vec{q}'$. If $\gamma_2(\vec{q}')$ is negative (or has scaled to a negative value), then the second term has the effect of slowing the decrease of $\gamma_1(\vec{q}_0)$ relative to other q values. Eventually $\gamma_1(\vec{q}_0)$ becomes equal for all $\vec{q}$, at which point the second term in Eq. (3.5) is unimportant and one scales to the $\gamma_1(\vec{q})=0$ fixed point. On the other hand, if $\gamma_2(\vec{q}')$ remains positive on the average, when $\gamma_1(\vec{q}_0)$ scales to zero the second term in Eq. (3.5) may remain positive. Thus $\gamma_1(\vec{q}_0)$ would scale from positive to negative. Once $\gamma_1(\vec{q}_0)$ becomes negative and reasonably large in magnitude the first term in Eq. (3.5) dominates and we scale on to the strong-coupling attractive fixed point discussed in detail by Mihaly and Solyom.[14] In particular, Eq. (3.5) is satisfied by

$$\gamma_1(\vec{q}) = [-2\xi + \gamma_1^{-1}(\xi=0,\vec{q})]^{-1}, \tag{3.7}$$

if only the first term on the right-hand side is kept. This implies that $\gamma_1(\vec{q}_0)$ diverges at some ξ. The interaction becomes long range in real space and a mean-field-type phase transition is predicted. Thus it is clear that the fixed-point behavior one scales onto depends strongly on the value of $\gamma_2(\vec{q})$. If $\gamma_2(\vec{q})$ is small or negative, one would scale onto the weak-coupling regime whereas for $\gamma_2(\vec{q})$ large and positive, one would scale onto the attractive strong-coupling regime even for repulsive initial $\gamma_1(\vec{q})$. In particular, from our results on the two-chain problem, we might speculate that if we start from a δ-function interaction $[\gamma_1(\vec{q})=\gamma_2(\vec{q})]$, irrespective of its sign, we will scale onto the attractive strong-coupling fixed point.

To verify the qualitative picture discussed above, we have solved the scaling equations (3.5) and (3.6) numerically. We take a one-dimensional array of chains and approximate the q values by a discrete set. Making use of the symmetry $\gamma_1(q) = \gamma_1(-q)$ and $\gamma_2(q)=\gamma_2(-q)$ we represent the functions γ_1 and γ_2 at nine discrete points between 0 and π/d, where d is the interchain spacing. This discretization clearly breaks down near the strong-coupling critical point when $\gamma_1(q)$ is rapidly varying. However, since we are mainly interested in the phase boundary which is determined by the scaling behavior relatively far away from the critical point, the discretization is not a bad approximation. For the same reason we do not expect the dimensionality to play a crucial role in determining the phase boundary, even though it would affect the critical behavior. Thus we chose a linear array of chains for simplicity. Furthermore, whether γ_1 scales through zero or not is determined by a scaling region in which the coupling constants are small and thus the first-order renormalization-group equations should be adequate.

We choose our starting Hamiltonian to consist of intrachain and nearest-neighbor coupling w_1 and w_2 only. For a variety of δ-function initial coupling constants that we tried we find that even when we start from a repulsive δ-function interaction, we scale to the attractive strong-coupling fixed point. Examination of the numerical solution shows that if we start from nearest-neighbor interactions, the interaction remains mostly nearest neighbor upon scaling until quite close to the transition. This suggests that the nearest-neighbor approximation studied in Sec. II should provide a good approximate picture for the phase diagram in coupling constant space. Specific numerical examples will be presented and discussed in Sec. V.

We should point out one significant difference between the two-chain and the N-chain problem. In the two-chain problem the attractive fixed point consists of g_1, g_2, w_1, w_2 all becoming infinite. Thus the interaction truly becomes attractive. In the N-chain case the divergence is in $\gamma_1(\vec{q})$ and the spatial representation of the coupling constants remains finite. In particular if we look at the coupling constant within the chain, we find that γ_2 may remain positive whereas γ_1 usually becomes small and negative. This kind of coupling constant can correspond to a repulsive interaction for two electrons on the same site and a stronger repulsion for two electrons on neighboring sites in the same chain.

Next we discuss briefly the situation when there are two types of chains in the system. Let us consider a one-dimensional array of alternating a and b type chains such that the spacing between a and b type chains is denoted by d. We will label chain a by odd indices and chain b by even indices. We shall assume that the Fermi velocity of the two chains is identical and define $\gamma^a_{1,i-j}$ and $\gamma^a_{2,i-j}$ as the coupling constants between the a chains and similarly for type b chains ($i-j$ is even) and γ^{ab}_{1i-j}, γ^{ab}_{2i-j} as the coupling constants between a and b chains ($i-j$ is odd). Again we go to Fourier space

$$\begin{aligned}\gamma_{1,a}(q)&=\sum_{k\ \text{even}} e^{ikq}\gamma^a_{1,k},\\ \gamma_{1,b}(q)&=\sum_{k\ \text{even}} e^{ikq}\gamma^b_{1,k},\\ \gamma_{1,ab}(q)&=\sum_{k\ \text{odd}} e^{ikq}\gamma^{ab}_{1,k}.\end{aligned}\tag{3.8}$$

Similarly we can define $\gamma_{2a}(q)$, $\gamma_{2b}(q)$, and $\gamma_{2ab}(q)$. The scaling equations are as follows:

$$\frac{d\gamma_{1a}(q)}{d\xi}=2\gamma^2_{1a}(q)+2\gamma^2_{1ab}(q)+2\sum_{q'}\gamma_{2a}(q-q')[\gamma_{1a}(q')-\gamma_{1a}(q)],\tag{3.9}$$

$$\frac{d\gamma_{1b}(q)}{d\xi}=2\gamma^2_{1b}(q)+2\gamma^2_{1ab}(q)+2\sum_{q'}\gamma_{2b}(q-q')[\gamma_{1b}(q)-\gamma_{1b}(q)],\tag{3.10}$$

$$\frac{d\gamma_{1ab}(q)}{d\xi}=2\gamma_{1ab}(q)[\gamma_{1a}(q)+\gamma_{1b}(q)]-\gamma_{1ab}(q)\sum_{q'}[\gamma_{2a}(q')+\gamma_{2b}(q')]+2\sum_{q'}\gamma_{1ab}(q')\gamma_{2ab}(q-q'),\tag{3.11}$$

$$\frac{d\gamma_{2\alpha}(q)}{d\xi}=\sum_{q'}\gamma_{1\alpha}(q-q')\gamma_{1\alpha}(q'),\quad \alpha=a,b\ \text{or}\ ab.\tag{3.12}$$

First we discuss the behavior near the strong-coupling fixed point. As in the equivalent chain case we neglect γ_2 relative to γ_1. Then the following approximate solutions:

$$\begin{aligned}\gamma_{1a}(q)&=[-2\xi+\tilde{\gamma}^{-1}_{1a}(q)]^{-1},\\ \gamma_{1ab}(q)&=[-2\xi+\tilde{\gamma}^{-1}_{1a}(q)]^{-1}\tilde{\gamma}_{1ab}\tilde{\gamma}^{-1}_{1a},\end{aligned}\tag{3.13}$$

and

$$\gamma_{1b}(q)=[-2\xi+\tilde{\gamma}^{-1}_{1a}(q)]^{-1}[\tilde{\gamma}_{1ab}\tilde{\gamma}^{-1}_{1a}]^2+\text{const}$$

are consistent in that $\gamma_{1a}(q)\gg\gamma_{1ab}(q)\gg\gamma_{1b}(q)$ for q near q_0 if the initial condition $\tilde{\gamma}_{1ab}\tilde{\gamma}^{-1}_{1a}$ is much less than one. Equations (3.13) are obtained by keeping only the leading term on the right-hand side of Eqs. (3.9)–(3.11). Thus we see that a mean-field-like transiton takes place simultaneously on both types of chains with the usual Ornstein-Zernike behavior. The power-law behavior obtained in Sec. II B for two inequivalent chains is then a special feature of the two-chain problem.

Finally, we should mention the special case when repulsive interaction between the type-a chain dominates. Then condensation is expected to take place at $q=\pi/2d$. For this value of q we see from Eq. (3.8) that $\gamma_{1,2ab}(q=\pi/2d)=0$. It is easy to see from the scaling equations that $\gamma_{1,2ab}(q=\pi/2d)$ remains zero upon scaling and that the a and b coupling constants are independent at this particular q value. Thus it is possible for a phase transition to take place on the type-a chain alone. In this case the problem reduces to that of the equivalent chains discussed earlier. Once the a chains are ordered it is possible for a distortion to be driven in the b chain at some lower temperature.[17]

IV. RESPONSE FUNCTIONS

In this section we discuss in turn the response function of the system at momentum transfer of $2k_F$, 0, and $4k_F$. We shall investigate the power-law behavior of the response functions at zero temperature and finite frequency by the renormalization-group method, keeping in mind the fact that $\max(\omega, T, vk)$ can be substituted for ω. Thus our results can be interpreted as the zero-frequency response at finite temperatures. The response function is defined by

$$R_{ij}(k,\omega)=-i\int dt\,dz\,e^{i\omega t}e^{-ikz}\times\langle T[O^\dagger(z,\vec{r}_i,t)\,O(0,\vec{r}_j,0)]\rangle \tag{4.1}$$

and

$$R(k,\vec{q},\omega)=\frac{1}{N}\sum_{ij}e^{-i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}R_{ij}(k,\omega),$$

where O is some two-particle or four-particle operator.

A. $2k_F$ and superconducting response functions

It has long been recognized that the one-dimensional electron gas has logarithmic singularities in its $2k_F$ response functions even in the noninteracting limit. Interaction enhances some of the response functions and suppresses others depending on the coupling constant. For the single-chain problem the following response functions have been investigated[7-10]:

(i) charge-density wave (CDW) response: $N(k,\vec{q},\omega)$

$$O(z,\vec{r}_i)=\sum_\sigma \psi^\dagger_{i1\sigma}(z)\,\psi_{i2\sigma}(z), \tag{4.2}$$

where

$$\psi_{i1\sigma}(z)=\sum_k e^{i(k_F+k)z}\alpha_{i\sigma}(k),$$

$$\psi_{i2\sigma}(z)=\sum_k e^{i(-k_F+k)z}\beta_{i\sigma}(k)$$

are the spatial representations of the electron annihilation operator on each side of the Fermi surface;

(ii) spin-density wave (SDW) response: $\chi(k,\vec{q},\omega)$

$$O(z,\vec{r}_i)=\psi^\dagger_{i1\uparrow}(z)\,\psi_{i2\downarrow}(z)-\psi^\dagger_{i1\downarrow}(z)\,\psi_{i2\uparrow}(z); \tag{4.3}$$

(iii) singlet-superconductor response: $\Delta_S(k,\vec{q},\omega)$:

$$O(z,\vec{r}_i)=\psi^\dagger_{i1\uparrow}(z)\,\psi^\dagger_{i2\downarrow}(z)+\psi^\dagger_{i2\uparrow}(z)\,\psi^\dagger_{i1\downarrow}(z); \tag{4.4}$$

(iv) triplet-superconductor response: $\Delta_T(k,\vec{q},\omega)$

$$O(z,\vec{r}_i)=\psi^\dagger_{i1\uparrow}(z)\,\psi^\dagger_{i2\downarrow}(z)-\psi^\dagger_{i2\uparrow}(z)\,\psi^\dagger_{i1\downarrow}(z). \tag{4.5}$$

For the coupled-chain problem there are two other response functions that are of interest.

(v) Excitonic response: $X^{(\pm)}_{\sigma\sigma'}(k,q,\omega)$

$$O_{\sigma\sigma'}(z,\vec{r}_i)=\psi^\dagger_{i,1\sigma}\,\psi^\dagger_{i+1,2\sigma'}\pm\psi^\dagger_{i2\sigma}\,\psi^\dagger_{i+1,1\sigma'}. \tag{4.6}$$

As it is written, this response function actually describes superconducting pairing of a $+k_F$ electron with a $-k_F$ electron on a neighboring chain. We call it the excitonic response because we have in mind a model of the charge-transfer system in which alternating chains are described by an electron or a hole band and the Fermi surface is at the crossing of the bands. For simplicity we assume that the two bands have identical Fermi velocity

$$H=\sum_{\substack{p,\sigma\\ i\text{ odd}}}\epsilon_p a^\dagger_{ip\sigma}a_{ip\sigma}-\sum_{\substack{p,\sigma\\ i\text{ even}}}\epsilon_p c^\dagger_{ip\sigma}c_{ip\sigma} \tag{4.7}$$

where $a^\dagger_{ip\sigma}$ ($c^\dagger_{ip\sigma}$) creates an electron on the odd (even) chain. By viewing the even chains as hole chains we make the transformation

$$c_{ip\sigma}=b^\dagger_{i-p\sigma}. \tag{4.8}$$

It is easy to see that all the chains now have the same band energy. The interaction Hamiltonian among a or among b chains is unchanged but the coupling constant between a and b chains now has opposite sign. The problem now reduces to the N-chain problem discussed in Sec. III. In particular pairing between particles on neighboring chains as described by Eq. (4.6) in this model is actually a pairing of an electron and a hole on neighboring chains. This response function then describes the tendency towards an excitonic state. This can be seen by examining the ordered state that would result if these response functions were to diverge. These ordered states involve hybridization of the chains in one of several ways. If the spin indices are chosen to give a pairing of the electron and hole in a spin singlet state, then the ordered state with $\langle X^{(+)}_S\rangle\neq 0$ has a hybridized charge density in the region between the chains. Note that while the size of the energy gap in these excitonic phases does not involve the overlap integral between chains, any measurable order parameter will involve this overlap integral. For example, the change in charge density when $\langle X_S^{(+)}\rangle \neq 0$ is proportional to this overlap integral. This charge density is uniform along the chain direction and varies as the cosine of the phase parameter. The energy of the ordered state is independent of this phase parameter which in the present case is the relative phase of the wave functions on the two chains. However, the presence of a small amount of overlap is sufficient to select a particular phase as the ground state. A state with $\langle X_S^{(-)}\rangle \neq 0$ is of some interest since it corresponds to a state with nonzero current along the chain direction. Such orbital current states have been discussed previously in connection with exciton insulator phases[18] though in most cases they alternated in space. In the present problem, such currents are uniform along the chain axis but their magnitude depends on the overlap between next-nearest-neighbor molecules on different chains and should be small. This current-carrying state cannot be the ground state and is probably never stable but the enhancement of the $X^{(-)}$ response function may have implications for the conductivity in the fluctuation region. Owing to the small interchain overlap, such contribution is probably of no practical interest. Finally we note that the triplet-spin excitonic response functions are the spin-density and spin-current analogs of charge density and current states discussed above.

(vi) Interchain Cooper pairing: $A_{\sigma\sigma'}(k,\omega)$

$$O_{\sigma\sigma'}(z,r_i)=\psi^\dagger_{i,1,\sigma}\psi_{i+1,2,\sigma'}\,. \qquad (4.9)$$

As it is written, Eq. (4.9) describes a $2k_F$ CDW between neighboring chains. Again for the electron-hole model, this response function corresponds to the Cooper pairing of $a_{ik\sigma}$ and $c_{i+1k\sigma'}$ with a net momentum of $2k_F$. This novel pairing is called to our attention by Anderson who pointed out its close analogy with pion condensation.[19]

Following the suggestion of Zawadowski, Solyom has provided a simple procedure for calculating these $2k_F$ response functions which is easily generalized to the N-chain case. It is convenient to work in the spatial representation in the transverse direction. We then follow Solyom and assume that it is the auxiliary quantities $\overline{R}\sim\partial R/\partial\xi$ that satisfy scaling equations. We define

$$\overline{N}=\pi v\frac{\partial N}{\partial\xi}\,,\quad \overline{\chi}=2\pi v\,\frac{\partial\chi}{\partial\xi}\,,$$
$$\overline{\Delta}_{S(T)}=-\pi v\,\frac{\partial\Delta_{S(T)}}{\partial\xi}\,,\quad \overline{X}^{(\pm)}_{\sigma\sigma'}=-2\pi v\frac{\partial X^{(\pm)}_{\sigma\sigma'}}{\partial\xi}\,, \qquad (4.10)$$
$$\overline{A}_{\sigma\sigma'}=2\pi v\frac{\partial A_{\sigma\sigma'}}{\partial\xi}\,.$$

A straightforward lowest-order perturbation calculation of the response function leads to the following scaling equations:

$$\frac{\partial\ln\overline{N}_{ij}}{\partial\xi}=4\gamma_{1ij}-2\gamma_{2ii}\delta_{ij}\,, \qquad (4.11)$$

$$\frac{\partial\ln\overline{\chi}_{ij}}{\partial\xi}=-2\gamma_{2ii}\delta_{ij}\,, \qquad (4.12)$$

$$\frac{\partial\ln\overline{\Delta}_S}{\partial\xi}=2(\gamma_{1ii}+\gamma_{2ii})\delta_{ij}\,, \qquad (4.13)$$

$$\frac{\partial\ln\overline{\Delta}_T}{\partial\xi}=2(-\gamma_{1ii}+\gamma_{2ii})\delta_{ij}\,, \qquad (4.14)$$

$$\frac{\partial\ln\overline{X}^{(\pm)}_{\sigma\sigma'}}{\partial\xi}=2(\pm\gamma_{1ij}+\gamma_{2ij})\delta_{i+1,j}\,, \qquad (4.15)$$

$$\frac{\partial\ln\overline{A}_{\sigma\sigma'}}{\partial\xi}=-2\gamma_{2ij}\delta_{i+1,j}\,. \qquad (4.16)$$

The first thing to note is that except for $\overline{N}$, all other response functions involve a δ function in the chain index. We recall from Sec. III that singularity in the coupling constant γ_1 develops in $\vec{q}$ space, and that in real space the coupling constants remain finite. Thus it is clear that at the three-dimensional ordering temperature only the CDW response function develops a true singularity. This result is a simple consequence of the neglect of interchain particle and spin-exchange scattering, which means that the CDW is the only one that can take advantage of the interchain Coulomb interaction. The rest of the response functions remain basically one dimensional.

To illustrate this point we have numerically integrated the scaling equations to get $\overline{N}$, $\overline{\chi}$, and $\overline{X}^{(\pm)}$, starting from the initial condition that at $\omega=E_F$, $\xi=0$, and $\ln\overline{N}=\ln\overline{\chi}=\ln\overline{X}^{(\pm)}=0$. These results are then further integrated to give the response functions N, χ, and $X^{(\pm)}$. A specific numerical example will be discussed in Sec. V. Here we note a rather interesting feature that if one begins with a repulsive short-range intrachain interaction, the SDW response χ is more strongly enhanced than the CDW response N over a large temperature range. It is only very close to the transition that $N(\vec{q}=0)$ rapidly increases and becomes dominant. The reason for this is obvious from Eq. (4.11) as the initially positive γ_1 reduces the growth of N relative to χ. It is only when γ_1 changes from repulsive to attractive that N grows rapidly. Even at this temperature the growth of χ is not directly affected, as it is driven only by γ_2. That the SDW response should be dominant over a large temperature range if we begin with repulsive interactions is a rather general feature of these equations. We also note that the interchain Cooper response function is suppressed for attractive interchain particle-hole interactions. Even if we start from a repulsive interaction it will become weaker upon scaling and will not be strongly divergent.

B. Uniform response functions

The uniform response functions that are of interest are:

(i) $q = 0$ density-density response function which is related to the compressibility: $N_0(k, \vec{q}, \omega)$

$$O(z, \vec{r}_i) = \sum_{\sigma} [\psi^{\dagger}_{i1\sigma}(z)\psi_{i1\sigma}(z) + \psi^{\dagger}_{i2\sigma}(z)\psi_{i2\sigma}(z)] \qquad (4.17)$$

and (ii) $q = 0$ spin density response function which is proportional to the uniform spin susceptibility: $\chi_0(k, \vec{q}, \omega)$

$$O(z, \vec{r}_i) = \psi^{\dagger}_{i1\uparrow}\psi_{i1\downarrow} + \psi^{\dagger}_{i2\uparrow}\psi_{i2\downarrow} . \qquad (4.18)$$

These response functions have been studied in the single-chain case by Fukuyama, Rice, Varma, and Halperin[8] using the renormalization-group method. The uniform spin susceptibility for a single chain has been calculated by Dzyaloshinskii and Larkin[6] using Landau Fermi-liquid theory. The difficulty with the $q = 0$ response function is that it requires the evaluation of

$$D(p, \omega) = \sum_{k\nu} G(k, \nu) G(p - k, \omega - \nu),$$

which is well known to have different limits for q, $\omega \to 0$ depending on the ratio vq/ω and care must be exercised in a diagrammatic expansion. The difficulties are not present if one uses Landau Fermi-liquid theory to relate N_0 and χ_0 to vertex functions evaluated at the Fermi level. This latter method is more transparent and we shall use it here. For completeness, some details of this method are given in Appendix B. It is clear that the spin susceptibility correlation function must be diagonal in the chain index and the result is similar to the single-chain result of Dzyaloshinskii and Larkin

$$\lim_{k \to 0,\ \omega/k \to 0} \chi_0(k, \omega, T) = \chi^*_{00}[1 + \gamma_{1ii}(T)], \qquad (4.19)$$

where χ^*_{00} is the noninteracting uniform susceptibility computed with a renormalized Fermi velocity v^* given by

$$v^*/v = 1 - g_1/2\pi v \qquad (4.20)$$

to lowest order in g_1 and $\gamma_{1ii}(T) = g_1(\xi)/2\pi v^*$. Thus the susceptibility is directly related to the renormalized coupling constant γ_{1ii} within a chain. Equation (4.19) predicts that for a repulsive interaction the susceptibility is enhanced relative to the noninteracting Pauli value and that the enhancement should decrease with temperature. In fact, for the single-chain problem, γ_1 scales to zero at $T = 0$ and the susceptibility enhancement is given by the velocity renormalization only. Shiba[20] has calculated the zero-temperature susceptibility for the one-dimensional Hubbard model with arbitrary filling using the exact solution of Lieb and Wu.[21] In Eq. (4.19), γ_{1ii} goes to zero at $T = 0$ and we find that in the small $g_1/2\pi v$ limit χ^*_{00} agrees with Shiba's results. In fact it appears that if we use a linear correction to the effective mass instead of the velocity as in Eq. (4.20), the agreement is maintained out to $g_1/2\pi v \approx 1$. For the N-chain case we find a similar decrease in the susceptibility enhancement. The new feature is that near the transition temperature γ_{1ii} can become negative and the susceptibility is further reduced. In Fig. 5 we show the behavior of γ_{1ii} obtained by numerical integration of the scaling equation.

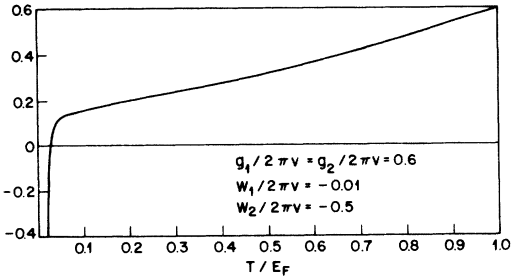

FIG. 5. Plot of γ_{1ii}, the intrachain coupling constant vs T/E_F.

Finally we discuss the compressibility. For the single-chain problem Fukuyama *et al.*[8] have shown that there is no logarithmic correction for the compressibility. The equation analogous to (4.19) for the density-density response function in the chain representation is

$$\lim_{k \to 0,\ \omega/k \to 0} N_{0ij}(k, \omega, T)$$

$$= N^*_{00}\left[1 + \left(\gamma_{1ij}\delta_{ij} - 2\sum_{j} \gamma_{2ij}\right)\right], \qquad (4.21)$$

where N^*_{00} is the noninteracting compressibility computed with v^*. It is clear from Eqs. (3.1) and (3.2) that the combination of the coupling constants on the right-hand side of Eq. (4.21) is invariant upon scaling. (In the single-chain case this reduces to the invariant $\gamma_1 - 2\gamma_2$.) Thus the compressibility remains unrenormalized.

C. $4k_F$ response

To obtain a response function at $4k_F$ we have to consider four-particle correlation functions. Two cases are of interest:

(i) $4k_F$ charge density wave $\Pi(4k_F+k,\vec{q},\omega)$,

$$O(z,\vec{r}_i)=\psi^\dagger_{2i\downarrow}\psi^\dagger_{2i\uparrow}\psi_{1i\uparrow}\psi_{1i\downarrow}. \tag{4.22}$$

(ii)

$$O(z,\vec{r}_i)=\psi^\dagger_{2i\sigma}\psi^\dagger_{2i+1\sigma'}\psi_{1i+1\sigma'}\psi_{1i\sigma}. \tag{4.23}$$

Just as in the case of interchain Cooper pairing, case (ii) is expected to be enhanced only for attractive interchain interactions between electrons. We shall focus our attention on case (i).

The $4k_F$ density-wave response function was first studied by Emery.[22] It differs from the $2k_F$ ones in a fundamental way. Whereas the $2k_F$ response functions are logarithmically divergent even for noninteracting systems, the $4k_F$ ones are not. Indeed it is easily seen that $\Pi(4k_F,\omega)\sim\text{const}+\omega^2\ln\omega/\epsilon_F$. This is because $4k_F$ response is basically a convolution of two $2k_F$ responses and the ω^2 factor comes from the extra momentum and frequency integral. First let us consider the single-chain problem. Examination of the perturbation series shows that it is of the form

$$\Pi(4k_F)\sim\text{const}+\omega^2\tilde{\Pi}/32\pi^3v^3,$$

where

$$\tilde{\Pi}=\xi+2[(g_1-2g_2)/2\pi v]\xi^2+\cdots. \tag{4.24}$$

The derivation of Eq. (4.24) can be found in Appendix C. It is natural to assume that $\tilde{\Pi}$ plays the same role as the $2k_F$ susceptibilities and we assume that $d\tilde{\Pi}/d\xi$ is the quantity that satisfies the scaling condition. We then obtain a power-law behavior for $\Pi(4k_F)$ in the usual way

$$\Pi(4k_F,\omega)\propto(\omega/E_F)^{2+4(g_1-2g_2)/2\pi v}.$$

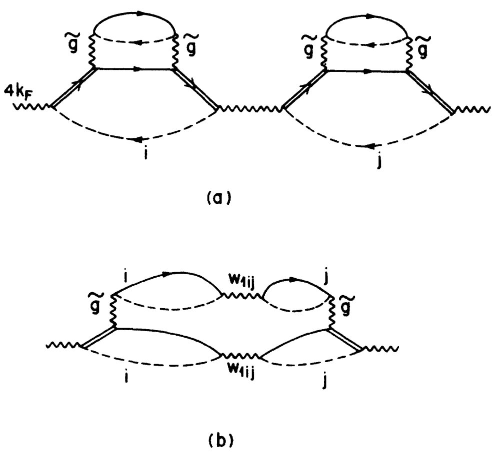

FIG. 6. Examples of diagrammatic contributions to the $4k_F$ response function. (a) Double line denotes as electron with momentum near $3k_F$. (b) Example of interchain coupling that is second order in w_{1ij}.

Owing to the presence of the ω^2 term, a large negative value for $(g_1-2g_2)/2\pi v$ is required for $\Pi(4k_F)$ to be divergent.

Before we discuss the N-chain problem, we consider the possible ways of coupling to a $4k_F$ excitation starting with two-particle interactions only. The natural way is to first excite an electron to an intermediate state near $3k_F$ as indicated in Fig. 6(a). Denoting the coupling constant by $\tilde{g}$ the coupling to $4k_F$ density fluctuations will be reduced by the factor $(\tilde{g}/D)^2$ where D is an energy denominator corresponding to the $3k_F$ intermediate state. We note that for a tight-binding band, depending on the value of $2k_F$, D may be a small fraction of E_F and $\tilde{g}/D$ may not be too small.

Now we discuss the effect of interchain coupling. Just as for the $2k_F$ charge-density wave the most important interaction is that which couples charge-density waves on different chains. There are two different ways in which the interchain coupling can occur. The first is depicted in Fig. 6(a) and is simply the Hartree coupling of the $4k_F$ charge-density waves. Note that the coupling is first order in the interchain interaction, but involves intermediate states in the electrons that can be far away from the Fermi surface. If this coupling is strong, we can have a locking of the $4k_F$ CDW on different chains. However, as discussed below we expect this coupling constant to be weak, in which case the CDW will remain uncorrelated from chain to chain until a lower temperature at which the $2k_F$ CDW begins to order three dimensionally. In this case a second process depicted in Fig. 6(b) becomes important. Note that this process is at least second order in w_{1ij}. However, near the three-dimensional transition for the $2k_F$ CDW w_{1ij} becomes relatively strong and long range and this second process may dominate. As a rough approximation we can assume that

$$\Pi_{ij}(4k_F)\approx(N_{ij})^2$$

near the three-dimensional transition temperature. Then if $N(q)$ is developing a pole at $q-q_0$, $\Pi(4k_F,q)$ will develop a pole at $q=2q_0$ and will appear as a harmonic of the $2k_F$ distortion.

V. DISCUSSION

In this paper we have studied the behavior of an array of one-dimensional metallic chains under the influence of interchain interactions. The most interesting conclusion is that even when the bare interaction is short range and repulsive, as the temperature is lowered the problem scales onto the fixed point corresponding to strong attractive coupling leading eventually to a three-dimensional phase transition into the CDW state. This behavior is in fact not too unexpected, if we remember that for the single-chain problem, when $g_1 - 2g_2 < 0$ the CDW and SDW response functions diverge with the same negative exponent. This is in contrast to the Hartree-Fock result which states the SDW is enhanced while CDW is suppressed. This rather surprising result arises because the diagram giving rise to the Hartree-Fock singularity is exactly cancelled by a graph in the Cooper channel. Thus for the single-chain problem we already have the rather surprising result that CDW response is divergent even for a repulsive short-range interaction. Now if we couple the chains together, and use mean-field theory to describe the interchain interaction, it is obvious that the CDW response will diverge at some transition temperature whereas the SDW response will be unaffected. The renormalization-group theory that we carried out here is nothing more than a proper mean-field theory for the coupled-chain problem and it is not surprising that we find a divergent CDW response with the additional feature that the coupling constant g_1 becomes large and negative in a region of momentum space. The reader may prefer to think of this change from repulsive to attractive attraction as "screening" by the interchain interaction. However, we emphasize that the "screening" process is in fact much more complicated than the usual mean-field theory involving particle-hole excitation and is a special consequence of the one-dimensional problem.

We next discuss the application of this model to organic conductors, of which TTF-TCNQ is a prototype. These are charge-transfer salts in which sheets of donor and acceptor stacks alternate in the $\vec{a}$ direction. The donor and acceptor bands are clearly not the same, but a model of alternating electron and hole bands with the same Fermi velocity and intrachain coupling constants is adequate as a starting point. The importance of intrachain Coulomb repulsion in the organic conductors was first pointed out by Torrance[23-25] and by Ovchinnikov[26] and co-workers. We estimate the coupling constants as follows:

$$\gamma_{1ij} = \frac{1}{2\pi v} \int dz\, V[z^2 + (x_i - x_j)^2] e^{i2k_F z}, \tag{5.1}$$

$$\gamma_{2ij} = \frac{1}{2\pi v} \int dz\, V[z^2 + (x_i - x_j)^2], \tag{5.2}$$

where $V(r^2)$ is the interaction potential in real space. We start with the Coulomb potential $V(r^2) = e^2/\epsilon r$ where ϵ is the high-frequency transverse dielectric constant in the conducting phase. For the estimate of γ_2 this Coulomb potential should be screened since screening at $q \approx 0$ is not logarithmically divergent and has not been included in our approach. To obtain an order-of-magnitude estimate we assume a screening length of one lattice constant in the b direction, we take $\epsilon = 6$ which is the measured low-temperature dielectric constant in the a direction,[27] and a bandwidth of 0.3 eV. The estimate for $\gamma_{2i,i+1}$ turns out to be of order unity. For

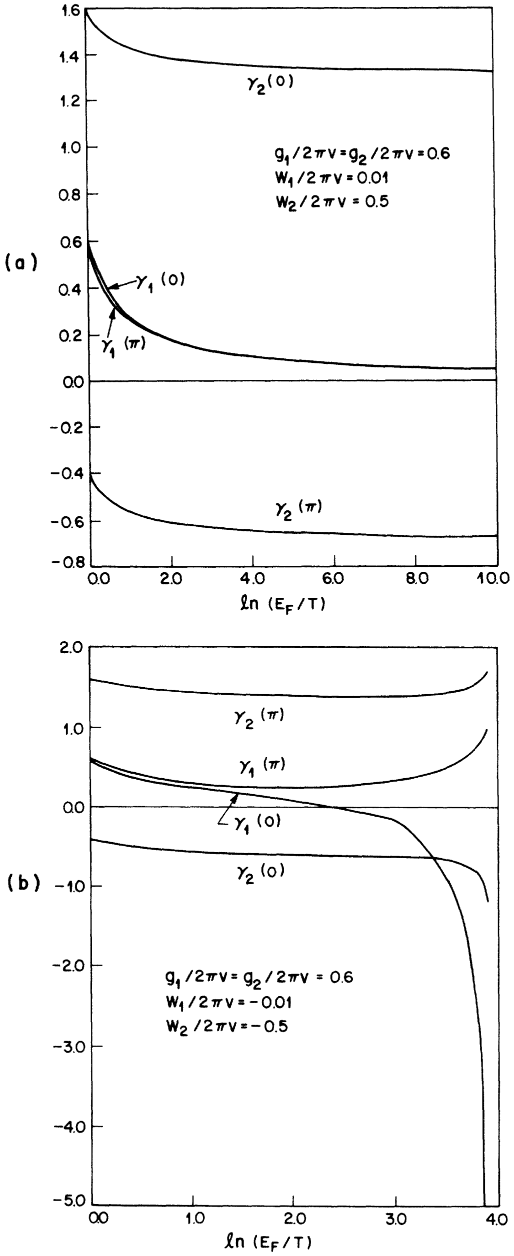

FIG. 7. Scaling behavior of the invariant coupling constants in momentum space, $\gamma_1(q=0)$, $\gamma_1(q=\pi/d)$, $\gamma_2(q=0)$, and $\gamma_2(q=\pi/d)$. (a) Scaling towards the weak coupling fixed point. Note that γ_1 becomes small and independent of q. (b) Scaling towards the attractive fixed point. Note that $\gamma_1(q=0)$ goes to $-\infty$ at some temperature.

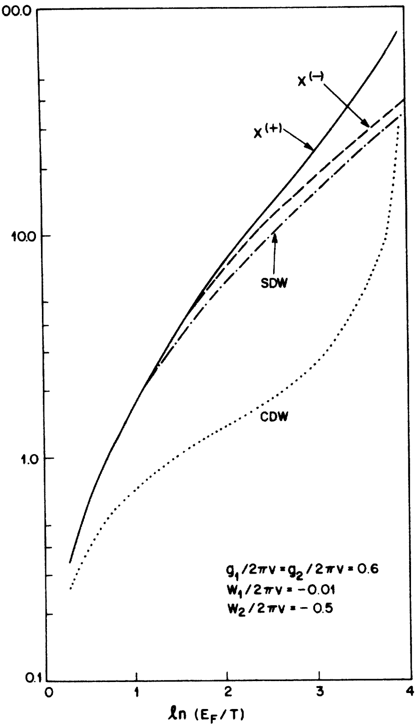

FIG. 8. Response functions corresponding to CDW, SDW, and $X^{(\pm)}$, the excitonic response, are plotted vs $\ln(E_F/T)$. Density of states factor $-(2\pi v)^{-1}$ for SDW and $X^{(\pm)}$ and $-(\pi v)^{-1}$ for CDW have been removed.

the intrachain coupling γ_{2ii}, it has been argued that two electrons on a TCNQ molecule tend to stay on opposite ends of the molecule and that there are large polarization effects. Both of these effects are unlikely to make γ_{2ii} smaller than the nearest-neighbor interchain coupling that we already estimated. Furthermore, since we assume a screening length of the order of a lattice constant, the interaction is short range and we conclude that $\gamma_{1ii} \approx \gamma_{2ii}$ are also of order unity. On the other hand

$$\gamma_{1i,i+1} \approx (1/2\pi v)(e^2/\epsilon)4K_0(2k_F d), \qquad (5.3)$$

where d is the spacing between stacks and $K_0(z) \sim (\pi/2z)^{1/2}e^{-z}$ is the Bessel function. We estimate $\gamma_{1i,i+1}$ to be of order 10^{-2}. This coupling constant is small because the potential between two sinusoidal charge-density waves decreases exponentially with the interchain spacing. In the rest of this section we shall discuss numerical results using the parameters $g_1/2\pi v = g_2/2\pi v = 0.6$, $w_1/2\pi v = \pm 10^{-2}$, and $w_2/2\pi v = \pm 0.5$ where the (+) sign should be used between identical chains and the (−) sign between donor and acceptor chains. In terms of the more familiar Hubbard notation, we note that for 0.59 electrons per atom, $g_1/2\pi v \approx 0.1U/t$.

Figure 7 shows the behavior of the renormalized coupling constants $\gamma_1(q=0)$, $\gamma_1(q=\pi/d)$, $\gamma_2(q=0)$, and $\gamma_2(q=\pi/d)$ for the two sets of initial coupling constants. We see that starting from $w_2/2\pi v = -0.5$ we scale onto the strong-coupling limit in which $\gamma_1(q=0)$ diverges whereas starting from $w_2/2\pi v = 0.5$, we scale to the weak-coupling limit. Again a rough criterion for the phase boundary in coupling constant space may be obtained by examining the two chain case. Since we start with a very small w_1, the only relevant criterion for scaling onto the weak-coupling limit is that $V > 0$ or $g_1 - 2g_2 + 2w_2 > 0$. Starting from a repulsive δ-function intrachain interaction it is clear that for $2w_2 < g$, which is satisfied for all negative and relatively small and positive w_2, we scale onto the strong-coupling fixed point. However, for $w_2/2\pi v = 0.5$ and $g/2\pi v = 0.6$, we scale to the weak-coupling limit as expected. At the same time we remark that for $w_2 < 0$, the transition temperature we obtain is enhanced over that predicted by a simple mean-field theory of interchain coupling. For example, in mean-field theory T_c is given by the condition[11,12]

$$1 - 2w_1\Pi(2k_F, T_c) = 0,$$

where $\Pi(2k_F)$ is the strictly one-dimensional density-density response function. The value of Π can be estimated from Fig. 8 by extrapolating the CDW result from the intermediate temperature region $[\ln(E_F/T) \approx 2]$ where the system is approximately one dimensional. It is clear that a much lower T_c will be obtained in this way. Thus the present theory suggests that there is a stronger tendency toward the locking of the donor and acceptor chains than the locking of similar chains. However, experimentally it appears that in TTF-TCNQ it is the TCNQ chains that first undergo a three-dimensional ordering which later drives a distortion in the TTF chains.[28,29] While this cannot be accounted for in our model in which the donor and acceptor chains are identical, it is easy to envision a situation in which interchain w_1 between TCNQ's are stronger than that between TTF and TCNQ, and that the Coulomb repulsion within each chain is different. In that case it is possible for sheets of TCNQ's to order first, which in turn leads to a three-dimensional ordering of the TCNQ sheets before driving a CDW on the TTF chains.

We next discuss the various physical properties based on our results on the correlation functions. It has been noted that the room-temperature magnetic susceptibility of TTF-TCNQ corresponds to a bandwidth of only ≈ 0.15 eV if the two chains are assumed to have similar bandwidth and consist of noninteracting electrons.[30] This bandwidth is less than the usual estimates and it has been suggested by Torrance and co-workers that the susceptibility is enhanced due to electron-electron repulsion.[24] Using Eq. (4.19) for the susceptibility we see from Fig. 5 that the susceptibility enhancement is slowly reduced as the temperature is lowered and the susceptibility drops off abruptly near the three-dimensional transition. If we interpret room temperature at roughly $T/E_F \approx 0.2$, we see that the gradual dropoff is too gentle to explain the experiments which drop by a factor of 2 between room temperature and 60 K. In practice electron-phonon interaction will enhance the growth of the CDW and might help explain the discrepancy.

As mentioned earlier the various divergent $2k_F$ response functions have been computed numerically and are shown in Fig. 8. We see that the CDW instability at $q=0$ is the only one that shows a real divergence at the three-dimensional transition temperature. For our choice of a large w_2, the excitonic responses $X^{(+)}$ and $X^{(-)}$ are strongly enhanced. This would imply a hybridization gap which will be strongly modified by fluctuation effects. The fluctuating gap appears as a self-energy correction in second-order renormalization-group theory and is not included in the present calculation. The physical interpretation of the enhancement of $X^{(+)}$ is that the wave functions on the two chains are developing coherence with respect to each other. In practice the direct observation of this coherence will be difficult, since the very small overlap of wave functions on neighboring chains will be involved. It is possible that the transverse conductivity will be enhanced as coherence develops in the transverse direction. However, in the absence of a satisfactory theory for the transverse conductivity, a convincing observation of the excitonic enhancement does not seem possible at the present time.

We next discuss the implication of the $2k_F$ CDW response function for dc conductivity in the chain direction. Let us consider the scattering of electrons by impurities. Quite generally the bare impurity potential V_0 is screened by the interacting electrons

$$V_s(q) = z_{k_F} \Lambda_4^{\infty}(q, k_F)\, V_0 \tag{5.4}$$

as discussed by Heine, Nozières, and Wilkins[31] within the Fermi-liquid theory. Here Λ_4^{∞} is the charge vertex function and z_{k_F} is the quasiparticle renormalization factor. To lowest order in g_1 and g_2 we have the expansion

$$V_0(2k_F) = V_0[1 + (2g_1 - g_2)\ln T/E_F + \cdots]. \tag{5.5}$$

As T is lowered from E_F, the second term in Eq. (5.5) screens out the bare potential. As T is further reduced, g_1 scales to zero and may become negative, at which point the impurity potential becomes enhanced. Since the scattering rate $1/\tau \propto [V_s(2k_F)]^2$, we expect a minimum of the scattering rate at some intermediate temperature. This point can be made more quantitative by the use of the memory function formalism[32,33] which gives

$$\frac{1}{\tau} = \lim_{\omega\to 0} \frac{c}{\omega} V_0^2 \sum_{kk'} \left(\frac{\partial\epsilon}{\partial k} - \frac{\partial\epsilon}{\partial k'}\right)^2 \operatorname{Im}\Pi(k-k', \omega), \tag{5.6}$$

where c is the impurity concentration and $\Pi(q)$ is the density-density response function. Clearly the main contribution in Eq. (5.6) comes from $k-k'$ near $2k_F$ where we have already calculated the real part of the response function $\operatorname{Re}\Pi(2k_F+q) = N(q)$. The imaginary part can be obtained by using the Kramers-Kronig relation from calculations of $N(\xi)$ shown in Fig. 8, for instance. We would like to make a rough estimate by assuming that

$$\operatorname{Re}\Pi(2k_F+q, \omega) = \begin{cases} N(q,T), & \omega < T, \\ a(\omega/E_F)^{-\nu(T)}, & \omega > T, \end{cases} \tag{5.7}$$

where the constant a is chosen so that $\operatorname{Re}\Pi(\omega)$ is continuous and

$$\nu(T) = -\frac{\partial \ln N}{\partial(\ln T/E_F)} = -\frac{1}{\pi v}\frac{\overline{N}}{N} \tag{5.8}$$

is the local slope in the logarithmic plot shown in Fig. 8. The Kramers-Kronig analysis can be done and it is easy to show that

$$\lim_{\omega\to 0} \frac{\operatorname{Im}\Pi(2k_F+q, \omega)}{\omega} = \frac{2}{\pi T}\frac{\nu}{\nu+1} N(q,T). \tag{5.9}$$

If $\nu \ll 1$ we obtain using Eqs. (5.6), (5.8), and (5.9):

$$1/\tau = cV_0^2(2/\pi)^2 \overline{N}(q=0, T), \tag{5.10}$$

where we have performed the sum over q by assuming that $\overline{N}(q)$ extends only over the range $|vq| < T$. It is amusing to note that the lowest-order expansion in g_1, g_2 of $\overline{N}$ agree with that of $[V_0(2k_F)]^2$ given in Eq. (5.5).

In the strictly one-dimensional case $\overline{N}(T)$ has been given by Solyom[7] within the lowest-order renormalization-group theory

$$\overline{N}(T) = [1 - (g_1/\pi v)\ln(T/E_F)]^{-3/2}(T/E_F)^{\alpha}, \tag{5.11}$$

where $\alpha = (g_1 - 2g_2)/2\pi v$. It is easy to show that a minimum occurs in $\overline{N}$ at a temperature $T_{\min}$ given by

$$\ln\frac{T_{\min}}{E_F} = \frac{2g_1 - g_2}{(g_1 - 2g_2)g_1} \tag{5.12}$$

and that the minimum value of $\overline{N}$ is

$$\bar{N}_{\min} = (-\alpha/3g_1)^{3/2} \exp[\tfrac{3}{2} + \tfrac{1}{2}(\alpha/g_1)]. \qquad (5.13)$$

For $g_1 = g_2$, $\bar{N}_{\min} = 0.523$ independent of g_1. When interchain coupling is included we find that the chains behave as if they are one dimensional over a wide temperature range and for the parameters chosen in Fig. 8, $\bar{N}_{\min}$ and $T_{\min}$ are in reasonable agreement with the one-dimensional result. It is of course possible to obtain a smaller $\bar{N}_{\min}$ and a lower $T_{\min}$ by varying the parameters g_1, g_2 and thus obtain a deeper minimum in τ^{-1}. We might add that electron-phonon scattering for $T > \omega_D$ can be treated in the same way by assuming that the excitation of the phonons produces a fluctuating potential so that $V_0^2 \to \langle V_{\text{phonon}}^2 \rangle \propto kT$. To summarize, the conductivity at some intermediate temperature can show a more rapid rise with decreasing temperature that T^{-1} owing to the screening of the random potential. Moreover, at lower temperature when the CDW is strongly enhanced, the random potential is enhanced and the conductivity decreases.

The other interesting feature in Fig. 8 is that for our choice of the repulsive intrachain interaction the SDW response is much stronger than the CDW response over a large temperature range. The SDW response function averaged over all momentum transfer should be directly measurable by the nuclear-spin relaxation rate which is given by[34]

$$\frac{1}{T_1} = 2\left(\frac{g\mu_B}{2}\right)^2 \frac{kT}{\omega} \sum_q |A_q|^2 \chi''(q,\omega), \qquad (5.14)$$

where $A_q = \frac{8}{3}\pi g \mu_B \gamma_n |u_q(0)|^2$ and $u_q(0)$ is the wave function at the nuclear site and γ_n is the nuclear gyromagnetic ratio. In Eq. (5.14), χ'' is the imaginary part of the retarded spin-flip response function. It has been argued[35] that at relatively low temperature $T \ll E_F$, the absorption from q near $\pm 2k_F$ dominates the sum in Eq. (5.14) and T_1^{-1} should be a direct measurement of the $2k_F$ SDW response. The experimental observation that $(T_1T)^{-1}$ decreases with decreasing temperature and apparently satisfies the Korringa relation has been used as an argument that no SDW enhancement occurs and therefore the electrons are weakly interacting.[35] This contradicts the estimates of the coupling constants made here and as we shall see, makes the observation of $4k_F$ CDW difficult to understand. In fact more recent work[36-38] has suggested that $1/T_1T$ may be dominated by the small q behavior of $\chi''(q,\omega)$. This is because for $ql < 1$ where l is the mean-free path the response function is diffusive,[39] i.e.,

$$\chi''(q,\omega)/\omega \approx Dq^2/[\omega^2 + (Dq^2)^2], \qquad (5.15)$$

where the diffusion constant is, roughly speaking, $v_F l$. Insertion into Eq. (5.14) shows that in a strictly one-dimensional problem $1/T_1T$ is enhanced from the Korringa-type expression by the factor $(\omega D/v_F^2)^{-1/2}$ where a is the lattice constant. Of course the $\omega^{-1/2}$ singularity is cut off by spin-orbit scattering or by the interchain hopping rate. Some frequency dependence of $1/T_1T$ has in fact been observed.[36,37] It is thus likely that $(T_1T)^{-1}$ is dominated by the small q behavior of the spin-density response function and contains no direct information on the $2k_F$ SDW and hence the strength of the interaction.

Further support of the existence of strong Coulomb repulsion comes from the recent observation of diffuse x-ray scattering streaks at $4k_F$ in TTF-TCNQ,[40,41] which have a different temperature dependence from the scattering at $2k_F$.[42,43] Emery[22] has pointed out that a strong repulsive interaction can explain this observation. He calculated the $4k_F$ charge-density wave response function for a single chain and obtained the following power-law behavior:

$$\Pi(4k_F,\omega) \sim (\omega/E_F)^{\mu}, \qquad (5.16)$$

$$\mu = -2 + 4[1 + (g_1 - 2g_2)/2\pi v]^{1/2} \times [1 - (g_1 - 2g_2)/2\pi v]^{-1/2}. \qquad (5.17)$$

Our renormalization-group result agrees with this exponent to lowest order in $g_1 - 2g_2$. As we observed before if $\mu < 0$, the interaction must be strongly repulsive since it has to overcome the leading ω^2 term. If the $4k_F$ divergence is stronger than the $2k_F$, then a large repulsive interaction is required. It is worth remarking that for strong Coulomb repulsion, the SDW is strongly divergent and we already expect a $4k_F$ CDW to occur as a harmonic of two SDW responses. This has, for example, been observed in the SDW phase in chromium metal.[44] We also wish to emphasize that for repulsive interaction, a $4k_F$ CDW necessarily coexists with strong SDW enhancement. It is then useful to consider the limit of the strongly repulsive Hubbard model and provide the following simple physical picture. In the infinite repulsion limit no two electrons may occupy the same site and the spin degrees of freedom may be approximated by that of a Heisenberg antiferromagnet. Ovchinnikov[45] has already considered the $\frac{1}{4}$ filled band and concluded that in the presence of a sufficiently strong nearest-neighbor repulsion, an energy gap exists and a CDW develops. This CDW in fact has wave vector $4k_F$ and simply states that electrons are localized on every other site. This is physically reasonable as the nearest-neighbor repulsion may compensate for the energy cost of localization. It is amusing to note that a nearest-neighbor repulsion corresponds to $g_1 < g_2$ which favors a $4k_F$ CDW according to Eq. (5.17). In TTF-TCNQ the charge transfer is 0.59 per molecule and we are about 15% away from the $\frac{1}{4}$ filled situation. Then we may envision a structure in which electrons are localized on every other site with occasional "defects" where two adjacent sites are occupied. This picture is similar to the discommensuration idea proposed by McMillan[46] and would show up as a $4k_F$ periodicity in x-ray diffraction with strong harmonic contents. This structure would conduct by the hopping of "defects." The detailed behavior of the conductivity will obviously be complicated. As the temperature is lowered, the coupling constants are renormalized in the way discussed in this paper. Eventually the electrons pair up to form singlet pairs and a $2k_F$ CDW is formed. The physical behavior is similar to the spin-Peierls transition.[47]

In conclusion, we have studied a model of coupled chains in which electron-electron interaction alone is considered. The most important feature is that even if we start with strong repulsive Coulomb interaction on both donor and acceptor chains (which we believe to correspond to the physical situation in charge-transfer compounds), we find that eventually the ground state is a CDW state that is three-dimensionally ordered. Enhancement of the magnetic susceptibility from the noninteracting band value and some decrease of the enhancement factor with lowering temperature is predicted, even though the temperature dependence is not strong enough to explain the experimental result in TTF-TCNQ. Strong SDW enhancement is predicted over a wide temperature range. While SDW has not been observed it is also not contradicted by existing data. Finally a simple physical picture of the strong-coupling limit is presented which exhibits a $4k_F$ CDW and is conducting. It appears that a model with repulsive electron-electron interaction may form a useful starting point for understanding the organic metals.

ACKNOWLEDGMENT

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APPENDIX A: SPECIAL SOLUTION FOR TWO EQUIVALENT CHAINS

A special solution of Eqs. (2.7) can be found along the surface $UV = W^2$. Substituting in the first of Eq. (2.8) leads to the result

$$\frac{V\,dx}{dV} = \tfrac{1}{2}(1 - x), \tag{A1}$$

where as previously $x \equiv U/V$. This is a separable equation which can be integrated at once to give the relation

$$[(U - V)/(U_0 - V_0)]^2 = V/V_0, \tag{A2}$$

where U_0 and V_0 are constants. Introducing the additional variable $Z = U - V$ leads us to a separable differential equation for $Z(\xi)$,

$$\frac{dZ}{d\xi} = 2Z^2\left(\frac{V_0}{Z_0^2} Z + 1\right). \tag{A3}$$

This equation can be integrated to give $Z(\xi)$ and thus from Eq. (A2), $U(\xi)$, $V(\xi)$, and then $W(\xi)$.

The properties of the solution are as follows: (i) if $U_0 > 0$, $V_0 > 0$, and $U_0 > V_0$ then as $\xi \to -\infty$, $U \to 0$, $V \to 0$ but $U/V \to +\infty$ (this corresponds to scaling to infinity in Fig. 3); (ii) if $U_0 > 0$, $V_0 > 0$, and $U_0 < V_0$ then as $\xi \to -\infty$, $U \to 0$, and $V \to (U_0 - V_0)^2/V_0$ (i.e., solution scales to the origin in Fig. 3); (iii) if $U_0 < 0$ and $V_0 < 0$ then $U \to -\infty$ and $V \to -\infty$ for a negative finite value of ξ (i.e., solution scales to the attractive fixed point).

APPENDIX B: UNIFORM RESPONSE FUNCTIONS

Consider first the uniform magnetic susceptibility. Then quite generally we have

$$\chi_0(k, \vec{q}, \omega) = -i\left(\sum_{p,\nu} G(p,\nu)G(p+k,\omega+\nu) + \frac{i}{N}\sum_{i,j} e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} \sum_{p_1\nu_1 p_2\nu_2} G(p_1,\nu_1)G(p_1+k,\nu_1+\omega) \right.$$
$$\left. \times \Gamma^{(ij,ij)}_{\uparrow\downarrow,\uparrow\downarrow}(p_1, p_1+k; p_2, p_2-k)\, G(p_2,\nu_2)\, G(p_2-k,\nu_2-\omega)\right), \tag{B1}$$

where

$$\Gamma^{(ijlm)}_{\alpha\beta\gamma\delta} = \Gamma_{1ij}\delta_{\alpha\gamma}\delta_{\beta\delta}\delta_{il}\delta_{jm} - \Gamma_{2ij}\delta_{\alpha\delta}\delta_{\beta\delta}\delta_{im}\delta_{jl} \tag{B2}$$

is the vertex function. It is clear that when there is a spin flip at the vertex, only the single-chain vertex function $\Gamma^{(ii,ii)}$ enters in Eq. (B1). Thus $\chi_0(k, \vec{q}, \omega)$ is independent of q and involves only a single chain. The difficulty remains that an inte-

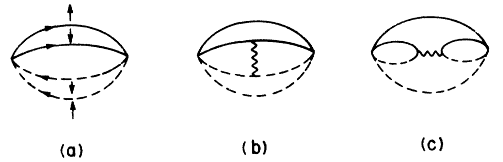

FIG. 9. Graphs that contribute to the $4k_F$ response function: (a) noninteracting response function, (b) a term proportional to g_2, and (c) a term proportional to g_1.

gration over the entire energy band is required in Eq. (B1). This difficulty is circumvented using techniques that are standard in Fermi-liquid theory.

The starting point is the observation that the Green's function can be written, near the Fermi level, as

$$G(k,\omega)=\frac{z}{\omega-v^*(|k|-k_F)+i\delta\,\mathrm{sgn}(|k|-k_F)}\,, \tag{B3}$$

where $v^*=v(1-g_1/2\pi v+\cdots)$ is the velocity normalization. (Strictly speaking in the bandwidth cutoff model of Menyhard and Solyom there is no velocity renormalization. However, such renormalization exists for the Hubbard model or for models with a cutoff in the momentum transfer.) We note that there are no logarithmic corrections to the velocity renormalization. Thus it is natural to perform the velocity renormalization first (i.e., v is replaced by v^* everywhere) and then sum the logarithmic terms using renormalization-group theory. The lowest-order logarithmic self-energy term shown in Fig. 5 of Ref. 7 has been shown by Menyhard and Solyom to correspond to a renormalization of z such that

$$z=[1-(4\pi^2v^{*2})^{-1}(g_1^2-g_1g_2+g_2^2)\ln(\omega/E_F)]^{-1}\,. \tag{B4}$$

In the Landau Fermi-liquid theory it has been shown in the long-wavelength limit that Eq. (B1) can be rewritten[48]

$$\lim_{k,\,\omega\to 0}\chi_0(k,\vec{q},\omega)=\frac{1}{2\pi v^*}\frac{kv^*}{\omega-kv^*}-\frac{1}{(2\pi v^*)^2}\frac{kv^*}{\omega-kv^*}\times z^2\Gamma^{ii,ii}_{\uparrow\downarrow,\uparrow\downarrow}(k_F,k_F,k_F,k_F)\frac{kv^*}{\omega-kv^*}\,. \tag{B5}$$

The important points are that the wave-function renormalization does not appear in the first term and that the second term is now evaluated only at the Fermi surface. The z^2 factor in the second term is now a higher-order correction which we ignore, and Γ evaluated at the Fermi surface can be written in terms of the renormalized coupling constants γ_1 and γ_2 defined as $g_1(\xi)/2\pi v^*$ and $g_2(\xi)/2\pi v^*$, respectively. This leads directly to Eq. (4.19). Similar consideration leads to Eq. (4.21) for the compressibility.

APPENDIX C: CHARGE-DENSITY-WAVE RESPONSE AT WAVE VECTOR $4k_F$

In this appendix we outline the calculation of the $4k_F$ charge-density-wave response function $\Pi(4k_F,\omega)$ of a single chain. First we consider the noninteracting response function $\Pi^0(4k_F,\omega)$, shown graphically in Fig. 9(a). By integrating over the internal variables associated with up- and down-spin lines one can obtain at once the result

$$\Pi^0(4k_F,i\omega)=\int\frac{du}{2\pi}\int\frac{dk}{2\pi}\,\Pi^0(2k_F+k,iu+i\omega)\times\Pi^0(2k_F-k,-iu)\,, \tag{C1}$$

where $\Pi^0(2k_F+k,iu)$ is the noninteracting $2k_F$ response function. It is convenient to evaluate all frequency integrals along the imaginary axis

$$\Pi^0(2k_F+k,iu)=\frac{1}{4\pi v}\ln\left(\frac{v^2k^2+u^2}{E_F^2}\right). \tag{C2}$$

The integrals in (C1) can be evaluated straightforwardly leading to

$$\Pi^0(4k_F,i\omega)=\text{const}-\frac{\omega^2}{32\pi^3v^3}\ln\left(\frac{\omega}{E_F}\right). \tag{C3}$$

The corrections of first order in the interaction are shown in Figs. 9(b) and 9(c). There are four graphs of type 9(b) involving g_2 but because of the restrictions imposed by the spin indices only two of type 9(c) involving g_1. Both types involve the same function $\Pi^{(1)}$ which has the form

$$\Pi^{(1)}(4k_F,i\omega)=\int\frac{du}{2\pi}\int\frac{dk}{2\pi}\,\Pi^0(2k_F+k,iu+\omega)\times[\Pi^0(2k_F-k,iu)]^2\,. \tag{C4}$$

Using the form (C2), one obtains

$$\Pi^{(1)}(4k_F,i\omega)=\frac{4E_F^2}{(4\pi)^5v^4}\times\int dy\,dx\,\ln[(x+\omega')^2+y^2]\ln^2(x^2+y^2)\,, \tag{C5}$$

where we have changed to variables $\omega'=\omega/E_F$, $x=u/E_F$, and $y=vk/E_F$. It is convenient to introduce polar coordinates $x=r\cos\theta$ and $y=r\sin\theta$. After integrating by parts and discarding an uninteresting constant we obtain

$$\Pi^{(1)} = -\frac{E_F^2}{(2\pi)^5 v^4}\int dr\left(\frac{r^2}{2}\ln^2 r - \frac{r^2}{2}\ln r + \frac{r^2}{4}\right)\int_0^\pi d\theta\,\frac{2r + 2\omega'\cos\theta}{r^2 + 2\omega'\cos\theta + \omega^2}$$

$$= -\frac{\pi E_F^2}{(2\pi)^5 v^4}\left[\int_{\omega'} dr\left(\frac{r}{2}\ln^2 r - \frac{r}{2}\ln r + \frac{r}{4}\right) - \int_0^{\omega'} dr\left(\frac{r}{2}\ln^2 r - \frac{r}{2}\ln r + \frac{r}{4}\right)\right] = \frac{\omega^2}{64\pi^4 v^4}\ln^2\frac{\omega}{E_F} + \cdots . \qquad \text{(C6)}$$

Finally we obtain the expansion

$$\Pi(4k_F, \omega) = \text{const} + \frac{1}{32\pi^3 v^3}\,\omega^2 \ln\frac{\omega}{E_F}\left(1 - \frac{4g_2 - 2g_1}{2\pi v}\ln\frac{\omega}{E_F} + \cdots\right). \qquad \text{(C7)}$$

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