

Theory of the quasi-one-dimensional electron gas with strong "on-site" interactions*

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It is shown that a quasi-one-dimensional system with strong attractive or repulsive coupling between electrons on the same site is equivalent to a Bose gas with hard core and longer-range interactions and to a Heisenberg-Ising magnet. Interchain and intrachain hopping and coupling are included and the equivalences are derived by elementary degenerate perturbation theory. Electronic correlation functions are derived from known pseudomagnetic ones and are used to discuss the circumstances in which superconductivity, charge- or spin-density wave transitions occur in the coupled chains.

I. INTRODUCTION

Quasi-one-dimensional systems typically consist of well-spaced chains of molecules for which the coupling of the electronic motion from one chain to another is relatively weak, and most of the interesting behavior takes place at temperatures T which are small compared to the scale temperature T_s for motions along the chain. Quantum-mechanical effects are important and, frequently, there are two types of correlation (e.g., superconductive and charge-density wave for metallic systems) which are coupled in an essential way. Any theory must, therefore, give an accurate account of the one-dimensional motion and the use of mean-field theory or classical fluctuations is likely to give misleading results. It is frequently possible to use mean-field theory for coupling *between* the chains because the long-range correlations which build up along the chains tend to suppress fluctuations,¹ but this still requires a good solution of the one-dimensional problem.

Of the methods proposed to deal with these systems, the renormalization group has been of limited use because, even when there is a phase transition and a fixed point of the Gell-Mann-Low equations, it occurs at an intermediate value of the coupling constant for which it is difficult to carry out accurate analytic calculations.² Using a different method Luther and Emery³ have found an exact solution of a quite general model for a particular value of one of the coupling constants and, with some imagination, the renormalization group may be used as a qualitative way of scaling onto other values. However, it is not always easy to calculate correlation functions and the inclusion of phonons in a dynamical way presents some problems. Moreover, the mathematical method, though not difficult, is not in common use, and this has led to expressions of doubt about some of the results. In particular, a question⁴ about the existence of an energy gap in the spin-density wave

spectrum for attractive interactions does not appear to be justified.^{5,6} Accordingly it would be useful to have an approach which uses relatively elementary methods and is easier to generalize. The purpose of this paper is to describe such a method. The ultimate objective is to include dynamical coupling to phonons, but for the present, in order to give a simple description and to make contact with previous results, a general static coupling between electrons will be adopted.

The main assumption is that the largest energy in the problem is the coupling U between electrons on the same molecule. This may be repulsive if Coulomb forces dominate or attractive if the molecule is very polarizable or, what amounts to the same thing, if there is strong coupling to intramolecular vibrations. It is quite likely that one or other of these situations is found in real physical systems, although this may only be realized *a posteriori*, when the results of calculations are compared to experiment.

The method is described in Sec. II. Elementary degenerate perturbation theory is used to take account of intrachain and interchain hopping of electrons and the coupling between electrons on different sites. It is shown that the effective Hamiltonian can be represented as either a set of bosons with hard cores and longer-ranged interactions or, more usefully, as a Heisenberg pseudospin system. For $U < 0$, the bosons are bound pairs of electrons and superconductivity occurs when they condense. In the spin picture, the pseudospin waves correspond to density waves and antiferromagnetic ordering in the z direction gives a charge-density wave state, whereas ferromagnetic ordering in the x - y plane is equivalent to a superconducting transition. The electron spin waves decouple from the charge-density waves and there is a gap in their energy spectrum as a consequence of pair breaking. This is analogous to the gap found by Luther and Emery.³ The pseudospin Hamiltonian has an anisotropic coupling stemming

partly from hopping and partly from direct electron coupling. It could be ferromagnetic or antiferromagnetic.

When the sign of U is reversed, the roles of charge- and spin-density waves are interchanged and there is a gap in the charge-density wave spectrum for the special case of a half-filled band. The pseudospins form an isotropically coupled antiferromagnet and ordering corresponds to a spin-density wave state of the original electron gas. These general conclusions agree with the results of Emery, Luther, and Peschel⁷ for an electron gas on a lattice, with intermediate repulsive coupling between electrons. In the absence of an interaction between electrons on different sites, the Hamiltonian is a generalization of the Hubbard model and, for $U > 0$, the equivalence to a Heisenberg antiferromagnet has been obtained previously by Anderson.⁸

In Sec. III, the electronic correlation functions are derived from those of the Heisenberg-Ising model and used to discuss long-range order in the ground state of a single chain and finite-temperature transitions in coupled chains. It is shown that hopping between chains can lead to any kind of transition but a density-density coupling leads only to a charge-density wave state. Superconductivity has the highest transition temperature only if the attractive electron-phonon coupling outweighs the Coulomb interaction between sites. Finally, the correlation functions and the method of calculating them are compared to those of the model of Luther and Emery.^{3,7}

II. LARGE ON-SITE COUPLING

It is assumed that the system consists of a set of chains of molecules providing a total of M sites for N electrons. The Hamiltonian is

$$H = H_0 + H_1 + H_2, \quad (2.1)$$

with

$$H_0 = U \sum_{i,\lambda} n_{\lambda i} n_{\lambda i}, \quad (2.2)$$

$$H_1 = \sum_{\substack{\lambda, \lambda' \\ i, j, \sigma}} t_{\lambda, i; \lambda', j} c_{\lambda i \sigma}^\dagger c_{\lambda' j \sigma}, \quad (2.3)$$

$$H_2 = \sum_{\substack{\lambda, \lambda' \\ i, j, \sigma, \sigma'}} V_{\lambda, i; \lambda', j} n_{\lambda i \sigma} n_{\lambda' j \sigma'}. \quad (2.4)$$

Here, λ, λ' identify the chains, i, j the sites along each chain, and $\sigma = \pm$ specifies the spins of the electrons. The $c_{\lambda i \sigma}^\dagger$ create electrons in states which are localized on the molecules and $n_{\lambda i \sigma}$ are the corresponding number operators. The hopping integrals $t_{\lambda, i; \lambda', j}$ and the coupling $V_{\lambda, i; \lambda', j}$ are as-

sumed to be zero for $\lambda = \lambda'$ and $i = j$, otherwise they are left unspecified. It is desirable to keep this general form since the geometric arrangement of molecules may allow the hopping and coupling between second and third neighbors along a chain to be comparable to that between electrons on molecules of different chains. The coupling in H_2 is a competition between Coulomb and electron-phonon interactions and its sign can vary from system to system. The largest energy is assumed to be U . If Coulomb interactions dominate $U > 0$; but very polarizable molecules, which also allow the electrons to be reasonably far apart, can have a reduced Coulomb interaction and a strong attractive attraction from intramolecular vibrations which, together, can lead to $U < 0$. Accordingly it will be sufficient to regard H_1 and H_2 as perturbations and to work to the lowest nontrivial order in H_1/U and H_2/U . It is simpler to separate the discussion of the two cases:

(a) $U < 0$: Here, the unperturbed ground state has $N/2$ of the sites occupied by pairs of opposite-spin electrons. These are real bound pairs which replace Cooper pairs⁹ in the strong coupling limit, although they are still responsible for superconductivity. When $N/2 < M$, the ground state is degenerate because the energy $NU/2$ is independent of which sites are occupied. The addition of H_0 and H_1 splits the degeneracy to form a band of charge-density wave states in which the pairs move from site to site. On the other hand, a spin-density excitation turns over a spin to break a pair at a cost $|U|$ in energy which (by assumption) is much larger than the bandwidth of the low-lying states. This energy gap causes the spin-density waves to be frozen out at low temperatures.

(b) $U > 0$: In this case the ground state has only one electron per site and it is degenerate because the energy does not depend upon which sites are occupied or upon the spins of the electrons. Once again, H_1 and H_2 split the degeneracy but there is no energy gap unless $N = M$ (half-filled band), when the excitation of charge-density waves is inevitably accompanied by double occupancy of sites at a cost in energy of at least $|U|$.

A more quantitative expression of this picture may be obtained from elementary degenerate perturbation theory. Attractive interactions, $U < 0$, will be considered first and it will then be shown how the results may be used for $U > 0$ without further calculation.

A. Attractive on-site interactions

The discussion will be restricted to the lowest band, in which all electrons remain paired. This is sufficient for a calculation of the low-tempera-

ture properties of the system. In first-order degenerate perturbation theory, $H_1 + H_2$ has to be diagonalized in the space of paired states and, within that space, it is an effective Hamiltonian from which the thermodynamic properties may be obtained. But H_1 breaks pairs and so has no first-order matrix elements. It must therefore be calculated to second order, allowing virtual transitions into the next band of states which have one pair broken. Suppose $H_2 = 0$ for the moment, and let the various degenerate ground states of H_0 be denoted by $|\alpha\rangle$ with energy $E_0 = NU/2$. The Schrödinger equation is

$$(E - H_0) |\psi\rangle = H_1 |\psi\rangle \quad (2.5)$$

and, dividing both sides by $E - H_0$ and rearranging, gives

$$|\psi\rangle = \sum_{\alpha} |\alpha\rangle \frac{\langle \alpha | H_1 | \psi \rangle}{E - E_0} + \frac{P}{E - H_0} H_1 |\psi\rangle, \quad (2.6)$$

where $P = 1 - \sum_{\alpha} |\alpha\rangle \langle \alpha|$ projects out of the unperturbed ground states. By substitution, it can be seen that Eq. (2.6) is equivalent to

$$|\psi\rangle = \sum_{\alpha} a_{\alpha} |\psi_{\alpha}\rangle, \quad (2.7)$$

where

$$|\psi_{\alpha}\rangle = |\alpha\rangle + [P/(E - H_0)] H_1 |\psi_{\alpha}\rangle \quad (2.8)$$

and

$$a_{\alpha} = \langle \alpha | H_1 | \psi \rangle / (E - E_0). \quad (2.9)$$

To first order, Eq. (2.8) is

$$\begin{aligned} |\psi_{\alpha}\rangle &= |\alpha\rangle + [P/(E - H_0)] H_1 |\alpha\rangle \\ &= |\alpha\rangle + (1/U) H_1 |\alpha\rangle. \end{aligned} \quad (2.10)$$

The last line follows because H_1 breaks exactly one pair to give an excitation energy $-U$ and P is irrelevant because $H_1 |\alpha\rangle$ has no component in the ground states. Then, substituting Eqs. (2.7) and (2.10) into Eq. (2.9) gives

$$(E - E_0) a_{\alpha} = \frac{1}{U} \sum_{\alpha'} \langle \alpha | H_1^2 | \alpha' \rangle a_{\alpha'}, \quad (2.11)$$

which is a Schrödinger equation in the $|\alpha\rangle$ subspace with effective Hamiltonian H_1^2/U . To ensure that H_1 acts between the ground states, it is necessary that if the first application of H_1 transfers an electron with spin σ from site j to site i , then the second application of H_1 either returns the electron to its original site or transfers an electron with spin $-\sigma$ from j to i . Thus, the effective Hamiltonian is

$$\begin{aligned} H_1^2 = - \sum_{\substack{\lambda, \lambda' \\ i, j, \sigma}} \frac{t_{\lambda, i; \lambda', j}^2}{|U|} (c_{\lambda i \sigma}^{\dagger} c_{\lambda' j \sigma} c_{\lambda' j \sigma}^{\dagger} c_{\lambda i \sigma} \\ + c_{\lambda i, -\sigma}^{\dagger} c_{\lambda' j, -\sigma} c_{\lambda i \sigma}^{\dagger} c_{\lambda' j \sigma}) \end{aligned} \quad (2.12)$$

Since it is sufficient to work to first order in H_2 ,

$$H' = H_1' + H_2 \quad (2.13)$$

is the total effective Hamiltonian which may be used to obtain the thermodynamic properties at temperatures $T \ll |U|$.

There are several equivalent ways of rewriting H' which relate it to more familiar systems. Define

$$n_{\lambda i} = \frac{1}{2}(n_{\lambda i+} + n_{\lambda i-} - 1), \quad (2.14)$$

$$b_{\lambda i} = c_{\lambda i+} c_{\lambda i-}, \quad (2.15)$$

$$\sigma_{\lambda i} = \frac{1}{2}(n_{\lambda i+} - n_{\lambda i-}). \quad (2.16)$$

Then

$$\begin{aligned} H' = \sum_{\substack{\lambda, \lambda' \\ i, j, \sigma}} \left(\frac{2t_{\lambda, i; \lambda', j}^2}{|U|} (-b_{\lambda i}^{\dagger} b_{\lambda' j} + n_{\lambda i} n_{\lambda' j} + \sigma_{\lambda i} \sigma_{\lambda' j} - \frac{1}{2}) \right. \\ \left. + V_{\lambda, i; \lambda', j} n_{\lambda i} n_{\lambda' j} \right). \end{aligned} \quad (2.17)$$

The operators $\sigma_{\lambda i}$ commute with the $b_{\lambda' j}$ and $n_{\lambda' j}$ and give zero acting on every doubly occupied site, so they are dynamically insignificant and will be ignored. The n_i and b_i satisfy the commutation relations

$$\begin{aligned} [b_{\lambda i}, b_{\lambda' j}^{\dagger}] = [b_{\lambda i}, b_{\lambda' j}] = 0, \quad i \neq j \\ b_{\lambda i}^2 = 0, \end{aligned} \quad (2.18)$$

$$[n_{\lambda i}, b_{\lambda' j}^{\dagger}] = b_{\lambda' j}^{\dagger} \delta_{ij} \delta_{\lambda \lambda'}.$$

It is then possible to interpret the $b_{\lambda i}$ as boson operators and the $n_{\lambda i}$ as the corresponding number operators, provided a hard-core interaction is added to ensure that at most one boson occupies each site. For a single chain, such a model has been considered by Schultz.¹⁰ The question of the existence of superconductivity in the original system is now rephrased as the existence of a condensation of the bosons. In the BCS theory of superconductivity,¹¹ the pairs of fermions condense into a macroscopic occupation of a zero-momentum state as they form whereas, in the strong-coupling limit, the formation of pairs and the condensation of their center-of-mass motion occurs independently. Indeed, for a single chain with only hard-core interactions, the ground state is composed entirely of pairs but there is no superconductivity because the bosons do not condense.¹⁰

A more useful representation of the system is obtained by noticing that Eqs. (2.18) are the commutation relations of spin- $\frac{1}{2}$ operators with the identification

$$b_{\lambda i} = s_{\lambda i}^-, \quad b_{\lambda i}^\dagger = s_{\lambda i}^+, \quad n_{\lambda i} = s_{\lambda i}^z, \quad (2.19)$$

where $s_{\lambda i}^\pm = s_{\lambda i}^x \pm s_{\lambda i}^y$. Comparison of Eqs. (2.14) and (2.19) shows that $s_{\lambda i}^z$ is +1 for a site occupied by a pair and -1 for an unoccupied site. As in the case of the Bose gas, it is much more convenient to carry out calculations in the grand canonical distribution, and since the number operator is essentially $\sum_{\lambda, i} s_{\lambda i}^z$, the chemical potential is an effective magnetic field and will be denoted by h . Then, in this representation,

$$H' = \sum_{\substack{\lambda, \lambda', \\ i, j, \sigma}} \left(\frac{2t_{\lambda, i; \lambda', j}^2}{|U|} (s_{\lambda i}^z s_{\lambda' j}^z - s_{\lambda i}^x s_{\lambda' j}^x - s_{\lambda i}^y s_{\lambda' j}^y) + V_{\lambda, i; \lambda', j} s_{\lambda i}^z s_{\lambda' j}^z - h \sum_{\lambda i} s_{\lambda i}^z \right) \quad (2.20)$$

and "spin-wave" excitations correspond to charge-density waves for the original electron system. In Sec. II B it will be shown that antiferromagnetic order in the z -components is equivalent to charge-density wave order in the electron gas and ferromagnetic order in the x - y direction represents condensation of the bosons or superconductivity of the electrons. The connection between the boson and the spin pictures is analogous to the pseudospin model of liquid helium.¹²

B. Repulsive on-site interactions

Turning now to the case $U > 0$, it will be assumed that $N = M$ (half-filled band), otherwise the hopping term H_1 breaks the degeneracy in first order by transferring an electron from a singly occupied site to an unoccupied site. This case is also of considerable physical interest. The effective Hamiltonian may be obtained directly from Eqs. (2.14)–(2.17) by making the canonical transformation

$$c_{\lambda i^-} = \bar{c}_{\lambda i^-}^\dagger, \quad c_{\lambda i^+} = \bar{c}_{\lambda i^+}, \quad (2.21)$$

for which

$$\bar{H}_0 = -U \sum_{i, \lambda} \bar{n}_{\lambda i^+} \bar{n}_{\lambda i^-} + U \sum_{i, \lambda} \bar{n}_{\lambda i^+}, \quad (2.22)$$

$$\bar{H}_1 = \sum_{\lambda, \lambda', i, j} t_{\lambda, i; \lambda', j} (\bar{c}_{\lambda i^+}^\dagger \bar{c}_{\lambda' j^+} - \bar{c}_{\lambda i^-}^\dagger \bar{c}_{\lambda' j^-}). \quad (2.23)$$

In the unperturbed states, sites which were occupied by an electron with $\sigma = -1$ are now empty whereas other sites are doubly occupied. The "on-site" coupling becomes attractive and the number of pairs is equal to the original number of spins with $\sigma = +1$. Second-order degenerate perturbation theory may now be used exactly as before and, on reversing the transformation (2.21), the effective Hamiltonian is given by Eq. (2.17) with the sign of the $b_{\lambda i}^\dagger b_{\lambda' j}$ term changed.

The variables have a rather different interpretation, since $b_{\lambda i}$ becomes $c_{\lambda i^+} c_{\lambda i^-}^\dagger$ and $\sigma_{\lambda i}$ replaces $n_{\lambda i}$ in the commutation relations (2.18) and in the relation to the spin operators in Eq. (2.19). Since every site is singly occupied, all of the $n_{\lambda i}$ give unity when applied to the ground states and so are dynamically insignificant. They will therefore be omitted and the effective spin Hamiltonian takes the antiferromagnetic, spin-isotropic, Heisenberg form:

$$H'' = \sum_{\lambda, \lambda', i, j} \frac{2t_{\lambda, i; \lambda', j}^2}{|U|} \bar{s}_{\lambda i} \cdot \bar{s}_{\lambda' j}. \quad (2.24)$$

There is no magnetic field because the number of electrons is fixed. The pseudospin-wave excitations are now true spin waves and changing the sign of U has interchanged the roles of charge- and spin-density excitations. This feature was found for a single chain by Emery, Luther, and Peschel⁷ when they obtained an exact solution for intermediate coupling. Because the original Hamiltonian had no direct spin-spin interaction, the exchange constants in Eq. (2.24) come entirely from the hopping term. For the repulsive Hubbard model, $U > 0$ and $H_2 = 0$, Eq. (2.24) has previously been obtained by Harris and Lange⁸ using a canonical transformation method.

III. CORRELATION FUNCTIONS

To discuss the existence of the various kinds of phase transition mentioned earlier, it is necessary to evaluate the correlation functions generated by $c_{\lambda i \sigma}^\dagger c_{\lambda' j \sigma'}$ or $c_{\lambda i \sigma} c_{\lambda' j \sigma'}$. When $U < 0$, the wave functions for the low-lying states are linear combinations of the $|\psi_\alpha\rangle$ of Eq. (2.10) which, in turn, are linear combinations of states with all sites occupied by pairs of electrons of opposite spin or with pairs broken without spin flip, and only $c_{\lambda i \pm}^\dagger c_{\lambda' j \pm}$ or $c_{\lambda i^+}^\dagger c_{\lambda' j^-}$ have matrix elements within this space. The other combinations connect to states in which there are unpaired electrons with parallel spins and are separated from the ground state by an energy gap $|U|$ which prevents divergences at zero frequency. This agrees with the conclusion of Lee.^{5,6}

To lowest order in $|t_{\lambda, i; \lambda', j}/U|$ it is sufficient to take $|\psi_\alpha\rangle \approx |\alpha\rangle$ and merely use H_1 and H_2 to determine the coefficients a_α for Eq. (2.7). Then only the operators

$$\frac{1}{2}(c_{\lambda i^+}^\dagger c_{\lambda i^+} + c_{\lambda i^-}^\dagger c_{\lambda i^-}) \equiv s_{\lambda i}^z + \frac{1}{2}, \quad (3.1)$$

$$c_{\lambda i^+}^\dagger c_{\lambda i^-}^\dagger \equiv s_{\lambda i}^+ \quad (3.2)$$

are relevant. In writing Eqs. (3.1) and (3.2) use has been made of Eqs. (2.14), (2.15), and (2.19). Since $\sigma_{\lambda i}$ commutes with the other operators, the

$c_{\lambda i \pm}^\dagger c_{\lambda i \pm}$ and $c_{\lambda i \pm}^\dagger c_{\lambda i \mp}$ correlation functions are equivalent to the $s_{\lambda i}^z$ and $s_{\lambda i}^x$ correlation functions of the spin representation of H' as asserted earlier. A charge-density wave then corresponds to antiferromagnetic ordering of the $s_{\lambda i}^z$, with the wave vector of the condensation determined by the applied field which represents the chemical potential. Similarly, superconductivity corresponds to ferromagnetic ordering in the $s_{i\lambda}^x$ and $s_{i\lambda}^y$ variables.

A similar argument may be made for $U > 0$. Starting from a half-filled band, $c_{\lambda i \pm}^\dagger c_{\lambda' j \mp}$ create states in which sites are doubly occupied at a cost of energy $2|U|$ relative to the ground state. The ordering variables are

$$s_{\lambda i}^* \equiv c_{\lambda i} - c_{\lambda i}^\dagger \quad (3.3)$$

and

$$s_{\lambda i}^z \equiv \sigma_{\lambda i} = \frac{1}{2}(c_{\lambda i}^\dagger c_{\lambda i} + c_{\lambda i} - c_{\lambda i}^\dagger), \quad (3.4)$$

which correspond to transverse and longitudinal spin-density waves, consistent with the spin isotropy of the Hamiltonian.

Given these representations, it is possible to make use of what is known about the Heisenberg-Ising model to calculate the properties of the electron system. The discussion will be restricted to the physically interesting case of near-neighbor coupling. First consider a single chain and choose units so that $2t_{\lambda i; \lambda, i+1}^2/|U| = 1$. Dropping the subscript λ , the contribution to the Hamiltonian from a single chain is, for $h=0$,

$$H_1 = - \sum_i (s_i^x s_{i+1}^x + s_i^y s_{i+1}^y + J_z s_i^z s_{i+1}^z). \quad (3.5)$$

Here, for $U > 0$, $J_z = -1$ gives the contribution to H'' in Eq. (2.24) after rotation of axes on alternate sites about the z direction and, for $U < 0$, the contribution to H' in Eq. (2.20) is obtained if

$$-J_z = V_{\lambda i; \lambda, i+1} + 1. \quad (3.6)$$

The case of greatest interest is $0 \geq J_z \geq -1$, for which the asymptotic forms of the correlation functions have been obtained by Luther and Peschel.¹³ It will be seen that this range is important for the discussion of the circumstances favorable to superconductivity. It is physically less realistic to have $J_z > 0$ because it requires a large attractive $V_{\lambda i; \lambda, i+1}$ and the pairs would form clusters in which adjacent sites were occupied. The properties for $J_z < -1$ may be obtained from the numerical calculations of Bonner and Fisher.¹⁴

The route followed by Luther and Peschel¹³ is to use a Jordan-Wigner transformation¹⁵ to rewrite H_1 as a fermion Hamiltonian and then to replace the kinetic energy by a linear spectrum to obtain a Luttinger model, for which it is relatively easy to obtain the correlation functions.¹⁶ If the site

label i is replaced by the distance r along the chain, then the asymptotic forms of the s^z and s^x correlation functions are given by¹³

$$\langle s^z(r, t) s^z \rangle = (2\pi^2 \alpha^2)^{-1} \cos 2k_F r \left(\frac{\alpha^2}{r^2 - c^2 t^2} \right)^{1/2 \theta} \quad (3.7)$$

and

$$\langle s^+(r, t) s^- \rangle + \langle s^-(r, t) s^+ \rangle = (2\pi^2 \alpha^2)^{-1} \left(\frac{\alpha^2}{r^2 - c^2 t^2} \right)^{\theta/2} \quad (3.8)$$

for $T=0$. Here, c is the Fermi velocity, t the time, α a cutoff, and

$$\theta = \frac{1}{2} - \pi^{-1} \arcsin J_z. \quad (3.9)$$

For large r , the correlation functions in Eqs. (3.7) and (3.8) fall off as $r^{-\theta-1}$ and $r^{-\theta}$, respectively, and since, according to Eq. (3.9), $\frac{1}{2} \leq \theta \leq 1$ when $0 \geq J_z \geq -1$, there is no long-range order in the ground state. This conclusion has been reached previously by Schultz¹⁰ for the special case¹⁷ $J_z = 0$, $\theta = \frac{1}{2}$, which corresponds to the Bose gas with hard-core interactions.

On the other hand, in a three-dimensional system, interchain coupling may produce long-range order at a finite temperature T_c . If T_c is small (in units of the exchange integral), it is possible to use mean-field theory for the interchain coupling provided the motion along the chains is treated accurately. Using Eqs. (3.7) and (3.8) together with the results of Ref. 1, Eq. (9),

$$T_c \sim |2t_{\lambda i; \lambda+1, i}^2/|U| + V_{\lambda i; \lambda+1, i}|^{1/(2-\theta^{-1})} \quad (3.10)$$

for a charge-density wave transition ($U < 0$), and

$$T_c \sim (2t_{\lambda i; \lambda+1, i}^2/|U|)^{1/(2-\theta)} \quad (3.11)$$

for superconductivity ($U < 0$) or a spin-density wave state ($U > 0$, $\theta = 1$). Note that the arguments in Eqs. (3.10) and (3.11) are small because they are interchain couplings in units of the intrachain exchange integral. It is clear that hopping between chains can drive any of the transitions but the density-density coupling $V_{\lambda i; \lambda+1, i}$ can give rise to a charge-density wave instability only.¹⁸ Equations (3.6) and (3.9)–(3.11) also show that if superconductivity is to occur at a higher temperature than the charge-density wave instability, the electron-phonon interaction must outweigh the Coulomb force to make $V_{\lambda i; \lambda' j}$ attractive. This would either decrease the argument of Eq. (3.10) or, more effectively, decrease θ .

It is interesting to compare these conclusions with previous calculations.^{3,7} The Fourier transforms of the correlation functions in Eqs. (3.7) and (3.8) are proportional to ω^μ , with μ equal to $\theta^{-1} - 2$ and $\theta - 2$, respectively. When $V_{\lambda i; \lambda, i+1} = 0$

as in Refs. 3 and 7, it follows from Eqs. (3.6) and (3.9) that $\mu = -1$ in both cases. This is in agreement with the results of Luther and Emery³ and Emery, Luther, and Peschel⁷ for a lattice model provided there is a half-filled band. In that case, in the low-temperature limit, when $U < 0$ backward scattering produces a gap in the spin-density wave spectrum and umklapp scattering renormalizes to zero the charge-density wave coupling v' which appears in Table I of Ref. 3. For $U > 0$, the roles of backward scattering and umklapp scattering and of charge-density and spin-density waves are interchanged. This does not mean that the special values of the coupling constants considered in Refs. 3 and 7 are effectively in the large- $|U|$ limit but, rather, for a half-filled band, the exponents are independent of U . It is necessary to keep this in mind in making comparisons with the phase diagrams for coupled chains obtained by Klemm and Gutfreund,¹⁸ which are rather different from those obtained here.

It is clear that the evaluation of the correlation functions is considerably simpler in the strong-coupling limit than in the case considered by Luther and Emery³ and Emery, Luther, and Peschel.⁷ It is also possible to work with more

general Hamiltonians. The reason for this is that H_1 in Eq. (3.5) is equivalent to a set of *spinless* fermions for which umklapp scattering and backward scattering do not play a particularly crucial role. In the model of Luther and Emery^{3,7} it is necessary to use a renormalization-group argument to deal with one or the other of these processes in calculating the exponents for an electron gas on a lattice, when there is a half-filled band. Also, numerical factors in the correlation functions involve boson representations of powers of fermion field operators, which are difficult to evaluate. Finally, Eqs. (3.7) and (3.8) give the correlation functions for the more general Hamiltonian (3.5), which includes the effects of direct near-neighbor coupling $V_{\lambda_i; \lambda_j}$ as well as hopping.

It is hoped that the general approach described in this paper is simple enough that it can give a description of the ordered states and be extended to include the dynamical effects of phonons. These topics are under investigation.

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¹⁷After this paper was submitted for publication, Dr. A. Zawadowski showed me a paper by K. V. Efetov and A. I. Larkin, *Zh. Eksp. Teor. Fiz.* **69**, 764 (1975) [English translation not yet available], who also considered the large- U limit and used the boson picture to obtain correlation functions for $J_z = 0$. The discussion of sound-wave excitations given in this paper is physically similar to that of Luther and Emery (Ref. 3) but omits umklapp scattering (Ref. 7), which has a significant effect on the conclusions.

¹⁸This has also been shown for intermediate coupling by R. A. Klemm and H. Gutfreund [*Phys. Rev. B* (to be published)], who also discussed the use of mean-field theory for coupling between the chains.