Superconductivity from Predominantly Repulsive Interactions in Quasi One-Dimensional Systems

G. T. Zimanyi[(a)] and S. A. Kivelson
Department of Physics, State University of New York at Stony Brook, Stony Brook, New York 11794

and

A. Luther
NORDITA, DK-2100, Copenhagen, Denmark
(Received 18 November 1987)

We show that for a one-dimensional electron gas with strong repulsive electron-electron interactions and a weak retarded attractive interaction, superconducting fluctuations can occur at high temperatures. The dominant driving force for these fluctuations is the repulsive interactions! Although the results are for a one-dimensional model, a strong analogy exists between our results and the short-ranged resonating-valence-bond picture of superconductivity.

PACS numbers: 74.20.−z, 74.70.Kn, 74.70.Vy

An old question which has been endowed with renewed urgency by the discovery of high-temperature superconductivity is whether superconductivity can arise from purely repulsive electron-electron interactions. This is particularly so in light of the delicate balance that exists in these materials between magnetism and superconductivity. In this note we summarize the results of a study of the properties of the one-dimensional electron gas with dominantly repulsive electron-electron interactions and weak, retarded attractive interactions. Our main results are as follows: (1) While divergent superconducting fluctuations do not arise in the purely repulsive model, the addition of even very weak time-retarded attractive interactions produces a strongly divergent superconducting susceptibility. Thus, the purely repulsive model is unstable in the renormalization-group sense to superconductivity; indeed, the larger the repulsion, the greater the superconducting susceptibility! (2) The 1D superconducting state is comprised of fluctuating valence bonds. (3) The excitations are solitons and reversed spin-charge relations. These results may shed some light on the resonating-valence-bond (RVB) state in 2D as well. (4) The effect is strongest for a nearly half-filled band, although it produces a dimerized insulator at exactly half filling; these results suggest that doped polyacetylene could support high-temperature superconductivity if material with fewer defects could be made.

The model we start with is the standard[1] continuum model of a one-dimensional electron gas with short-range (i.e., screened) electron-electron repulsions, and a nearly half-filled band. The one electron spectrum is linearized about the Fermi surface, so there are two flavors of electrons: right-moving electrons with k near k_F and left-moving electrons with k near $-k_F$. The parameters in the models are the Fermi velocity V_F, the chemical potential μ (chosen so that $\mu=0$ for a half-filled band), the bandwidth or ultraviolet cutoff $E_F \approx hV_F k_F$, and the scattering amplitudes for backward (with parallel or antiparallel spin), forward, umklapp, and the "one-branch" scatterings $g_{1\parallel}$, $g_{1\perp}$, g_2, g_3, and g_4, respectively.

For an extended Hubbard model, $g_{1\parallel}=g_{1\perp}=g_3=(U-2V)a$, and $g_2=g_4=(U+2V)a$. For any model which is spin-rotationally invariant, $g_{1\parallel}=g_{1\perp}$. Note, unlike many other workers, we treat the half-filled and non-half-filled bands on an equal footing by varying μ; for large μ, g_3 becomes unimportant. g_4 is always relatively unimportant; it simply produces a shift in the velocities of the spin and charge degrees of freedom, $V_c=V_F(1+g_4)$ and $V_s=V_F(1-g_4)$, respectively.

This model has been extensively studied and a variety of features of the solution are known. (i) So long as excitations involving states at the band edges can be ignored, the Hamiltonian can be reexpressed as the sum of a charge and spin part; all physical correlation functions are expressible as a product of a spin factor and a charge factor. (ii) In the perturbative expansion for different correlation functions, logarithmic singularities appear in every order. Therefore one has to sum up at least the most divergent contributions, e.g., by applying the multiplicative renormalization group (RG). We study the lowest-order scaling equations because they already establish the qualitative equivalence of the model with weak bare couplings to some solvable models. The RG flows are determined by our integrating out the states between E_F and E_F'. The following scaling equations are obtained so long as $E_F' \gg \mu$:

$$g_1' = (\pi V_s)^{-1} g_1^2, \tag{1a}$$

$$g_c' = (\pi V_c)^{-1} g_c^2, \tag{1b}$$

$$g_3' = (\pi V_c)^{-1} g_c g_3, \tag{1c}$$

where g_j' signifies a derivative of g_j with respect to $\ln(E_F')$ and $g_c = g_{1\parallel} - 2g_2$. [When E_F is of order μ, the scaling equations cross over to those of an incommensurate system, which are the same as those in Eqs. (1) with g_3 set equal to zero.] (iii) The spin-excitation spectrum

is gapless if $g_1 \geq 0$ and has a gap Δ_s if $g_1 < 0$. The charge-excitation spectrum is gapless if $g_c \geq |g_3|$ and has a gap Δ_c otherwise. However, the Fermi energy lies in the gap only so long as $|\mu| < \Delta_c$. (iv) The ground state has a divergent antiferromagnetic susceptibility if $\Delta_s = 0$ and $\Delta_c > 0$; it has a divergent singlet superconducting and/or charge-density wave (CDW) susceptibility if $\Delta_s > 0$ and it is not insulating. (v) The charge excitations are spinless solitons, which can be thought of as bosons with short-ranged repulsive interactions, and the spin excitations are massive, neutral solitons.

In the half-filled repulsive Hubbard model, antiferromagnetic fluctuations dominate over superconductivity, and even on doping the system fails to become superconducting. However, the following fact is conspicuous: The scaling trajectory for the spin degrees of freedom follows the separatrix between the $\Delta_s = 0$ and $\Delta_s > 0$ phases and eventually scales towards the unstable noninteracting fixed point $g_{1\parallel} = g_{1\perp} = 0$. Thus one suspects that a small additional attraction might make the trajectories enter the $\Delta_s > 0$ phase.

We consider the effect of a weak retarded attraction which could arise because of the coupling of the electrons to almost any other degrees of freedom, since second-order perturbation theory gives a negative contribution to the low-energy states. We consider explicitly two extreme models of electron-lattice coupling: (i) the Su, Schrieffer, and Heeger[2] (SSH) model, in which the lattice distortions modulate the electron-hopping matrix elements, which we will refer to as coupling to the bond charge, and (ii) the molecular-crystal[3] (MC) model, in which an optical phonon couples to the electron site energy. The phonon propagator takes the usual Bose form, $D(k,\omega) = \omega^2(k)/[\omega^2 - \omega^2(k)]$. For an SSH coupling, the coupling vanishes at zero momentum transfer, and so we can approximate the dispersion by its value at the zone boundary, $\omega(k) \approx \omega_0 \equiv \omega(2k_F)$. For the MC model also, we can approximate the optical-phonon dispersion by an Einstein oscillator. Thus D is roughly k independent and its frequency dependence can be approximated by $D(\omega) = -\theta(\omega_D - \omega)$.

Thus, we define[4] retarded interactions $\tilde{g}_j$ analogous to the instantaneous interactions g_j. For the SSH model, $-\tilde{g}_1 = \tilde{g}_3 > 0$ and $\tilde{g}_2 = 0$, while for the MC model, $-\tilde{g}_1 = -\tilde{g}_3 = -\tilde{g}_2 > 0$.

The one-loop scaling equations for this two-cutoff model can be derived simply; the instantaneous interactions g_j [Eqs. (1)] are unaffected by the presence of retarded interactions. The equations for the retarded interactions $\tilde{g}_j$ are

$$\tilde{g}_1' = (\pi V_F)^{-1}(\tfrac{3}{2} g_1 \tilde{g}_1 + g_3 \tilde{g}_3 + \tfrac{1}{2} g_c \tilde{g}_1 + \tilde{g}_1^2 + \tilde{g}_3^2), \quad (2a)$$

$$\tilde{g}_2' = 0, \quad (2b)$$

$$\tilde{g}_3' = (\pi V_F)^{-1}(\tfrac{3}{2} g_1 \tilde{g}_3 + g_3 \tilde{g}_1 + \tfrac{1}{2} g_c \tilde{g}_3 + 2\tilde{g}_1 \tilde{g}_3). \quad (2c)$$

These equations are our most important result. They differ from earlier results[4,5] by the presence of cross terms $g_j \tilde{g}_k$. The scaling equations for $\tilde{g}_1$ and $\tilde{g}_3$ can be combined to produce two separate scaling equations for $\tilde{g}_\pm = \tilde{g}_1 \pm \tilde{g}_3$:

$$\tilde{g}_\pm' (\pi V_F)^{-1}\{(\tfrac{3}{2} g_1 \pm g_3 + \tfrac{1}{2} g_c)\tilde{g}_\pm + \tilde{g}_\pm^2\}, \quad (3)$$

which implies, among other things, that if initially $\tilde{g}_1 = \pm \tilde{g}_3$, as it is for both the SSH and the MC models, this equality is preserved by the scaling equations. In addition, ω_D is renormalized because of the Peierls softening[1b]; for the SSH model,

$$\omega_D' = \omega_D (\pi V_F)^{-1} \tilde{g}_+. \quad (4)$$

There are several important consequences of Eqs. (2). A positive derivative implies that $\tilde{g}_j$ scales toward large negative values. For dominantly repulsive interactions, the cross terms are the most important, since $g_j > \tilde{g}_j$. For the SSH model, the first term[6] in Eq. (2a) is negative, while all the other terms are positive, while in Eq. (2c) the first term is positive and all others terms are negative. Thus, as g_1 scales to zero, and g_c and g_3 scale to larger magnitudes according to Eqs. (1), $\tilde{g}_1$, in particular, and $\tilde{g}_3$ scale to larger magnitudes at a rate which is proportional to the strength of the electron-electron repulsion.

The perturbative scaling equations break down when $\gamma_j \equiv g_j/\pi V_F$ gets to be of order 1, and even the notion of scaling equations becomes dubious; only in the vicinity of the fixed point at $g_j = 0$ can we safely ignore the irrelevant interactions that are generated as we integrate out the high-energy degrees of freedom. Faced with this, one traditionally notes that the value of E_F' at which g_j gets to be of order 1 is a characteristic energy of the problem which can roughly be identified as the gap Δ. In the present problem, a crossover in the scaling equations also occurs when $E_F' \sim \omega_0$, where ω_0, the physical phonon frequency, is defined by the expression $\omega_0 = \omega_D(\omega_0)$, where $\omega_D(E_F')$ is the renormalized value of ω_D. We discuss here the case where $\omega_0 > \Delta_s, \Delta_c$. (The case $\Delta_c > \omega_0$ will be treated elsewhere.[7]) When $E_F' \sim \omega_0$, g_j and $\tilde{g}_j$ represent practically the same scattering process, and we can approximately represent their combined action in terms of a single interaction

$$g_i^T = g_i(\omega_0) + \tilde{g}_i(\omega_0), \quad (5)$$

where $g_i(\omega_0)$ and $\tilde{g}_i(\omega_0)$ are obtained by integration of the scaling equations from E_F to ω_0. (There is also a small renormalization of the Fermi velocity which arises from our integrating out the states with $E_F \sim \omega_0$.) The result is that the properties of the system at energies small compared to ω_0 can be derived from a standard continuum model with interactions g^T and bandwidth ω_0.

Several important physical consequences of the scaling equations can be derived simply: (i) Even if the bare in-

teractions are dominantly repulsive (i.e., $g_1 \gg |\tilde{g}_1|$), if ω_0/E_F is sufficiently small, the low-energy properties of the system will correspond to a negative g_1^T. Thus, the system will have a nonzero spin gap and the possibility of divergent superconducting and CDW susceptibilities. (ii) Because of the decoupling of the spin and charge degrees of freedom, the gap in the spin-excitation spectrum is approximately independent of dopant concentration. (iii) Despite the fact that the low-energy properties are characteristic of attractive interactions, at high energies $E \gg \omega_0$ (or temperature), the fact that the bare interactions are repulsive implies that the antiferromagnetic susceptibility should be large.

To obtain explicit expressions for the correlation functions, we must find a model along the scaling trajectory which we can solve in a controlled approximation. Here we can only sketch the results. The appropriate excitation spectrum and the spin charge factors for each correlation function of the standard model can be related[1] (via bosonization) exactly to the solution of a massive Thirring model

$$H_{MT} = \int dx\, \psi^\dagger(x)[-iV_0\sigma_z\partial_x + \Delta_0\sigma_x + \mu_0]\psi(x) - g_0 \int dx\, \psi_1^\dagger(x)\psi_2^\dagger(x)\psi_2(x)\psi_1(x), \quad (6)$$

where for the spin degrees of freedom the parameters in H_{MT} take the values

$$V_0 = V_s = V_F \tfrac{5}{4}(1 + \tfrac{3}{10}\gamma_{1\parallel}), \quad \mu_0 = 0,$$

$$\Delta_0 = \Delta_s = E_F \gamma_{1\perp},$$

and

$$g_0/\pi V_F = \tfrac{3}{2}(1 + \tfrac{5}{6}\gamma_{1\parallel}),$$

while for the charge degrees of freedom,

$$V_0 = V_c = V_F \tfrac{5}{4}(1 + \gamma_4 + \tfrac{3}{10}\gamma_c), \quad \mu_0 = \mu,$$

$$\Delta_0 = \Delta_c = E_F\gamma_3, \quad g_0/\pi V_F = \tfrac{3}{2}(1 + \gamma_4 + \tfrac{5}{6}\gamma_c),$$

where $\gamma_j = g_j^T/\pi V_F$ are the dimensionless coupling constants. The spectrum of this model for $\mu_0 = 0$ has been computed exactly by the Bethe *Ansatz*; however, there are no exact expressions for the correlation functions.

In order to obtain the correlation functions of the system one would like to follow the scaling trajectories until they reach the solvable Luther-Emergy[8] model, where $g_0 = 0$. When one does so, additional interactions may arise, but their effect on the spin channel will be only perturbative in X, where

$$X = (g_0/2\pi V_F)\ln(E_F'/\Delta) \ll 1 \quad (7)$$

since the spectrum has a gap Δ_0. A similar statement holds for the charge channel with the difference that there is an additional set of excitations below the gap. To treat them we linearize the spectrum around μ [this gives a Fermi-velocity renormalization $V_0 = V_c(\mu - \Delta_c)/\Delta_c$] and this leads to a massless Thirring model (H_{MT} with $\Delta_0 = 0$) with bandwidth cutoff $E_F^* = |\mu| - \Delta_c$, which is solvable via bosonization. Taking over the known correlation functions,[1] we obtain for $T < \min\{\Delta_s, E_F^*\}$ the superconducting susceptibility

$$\chi_{SS} \sim \Delta_s^2 (E^*/kT)^{2-\Theta_c^{-1}}, \quad (8)$$

and the incommensurate CDW susceptibility

$$\chi_{CDW} \sim \Delta_s^2 (E^*/kT)^{2-\Theta_c}, \quad (9)$$

where the exponent is

$$\Theta_c = \left(\frac{1 + \gamma_4 + \frac{1}{2}\gamma_c}{1 + \gamma_4 - \frac{1}{2}\gamma_c}\right)^{1/2}. \quad (10)$$

The form of Eqs. (8) and (9) is ensured by the mapping to the Thirring model; however, our ability to calculate Θ_c quantitatively in terms of the parameters of the original model is limited. Since we must scale until $X < 1$ while $|\gamma_c| < 1$, hence $\frac{1}{2} < \Theta_c < 1$—the CDW susceptibility is thus the most divergent, but the superconducting susceptibility is comparably divergent. It is easy to see as well that the stronger the bare repulsive interactions, the larger Δ_s and so χ_{SS}. Δ_s depends only relatively weakly on the strength of the retarded interactions. To get a genuine superconducting transition we make the standard arguments that the presence of weak interchain coupling will cause a transition at a temperature at which χ_{SS} gets sufficiently large.

We now comment on the analogy between the present results and the resonating-valence-bond (RVB) theories of high-temperature superconductivity. Two classes of RVB states have been studied: (1) the original RVB state of Fazekas and Anderson[9] which is the prototypical short-range RVB state (SR-RVB) and was explicitly characterized in the context of superconductivity by Kivelson, Rokhsar, and Sethna[10]; (2) the generalized RVB state of Baskaran, Zou, and Anderson[11] which has all-length valence bonds. Both describe quantum spin-liquid states, but the former is thought to have a gap[10,12] to spin excitations while the latter is gapless. In either case, the spin excitations are neutral spin-$\frac{1}{2}$ solitons while the charged excitation are spinless.[10-12] For the half-filled band there is a Mott gap in the charge-excitation spectrum which is destroyed on doping. While the majority of the calculations involving the RVB state have been carried out for the simple Hubbard model, it has been realized from the outset[11] that weak additional interactions, e.g., further-neighbor interactions which frustrate the Néel state, or electron-phonon interactions, may be necessary to stabilize the RVB state. Thus, there is a close correspondence between the excitations of the RVB state and those of the one-dimensional electron gas with g_1^T, $g_c^T < 0$ and $g_3^T > 0$: The excitations are solitons with reversed charge-spin relations, there is a strong tendency toward superconductivity below the degeneracy

temperature of the holes (suggesting they are bosonlike), and the state is stabilized by electron-phonon coupling. As in the SR-RVB state, and in contradistinction to the Baskaran-Zou-Anderson state, there is a gap to spin excitations. Of course, for $g_1^T > 0$, the same reverse charge-spin relations exist but there is no gap in the spin-excitation spectrum; unfortunately, neither are there divergent superconducting fluctuations. This comparison lends modest support to the SR-RVB analysis in two dimensions; we stress, however, that resonance is very much more limited in one dimension than in two, and the gap could be dependent on dimensionality.

In another communication,[13] we discuss in detail the relevance of our results for actual quasi one-dimensional materials, especially doped polyacetylene. Here we conclude by making a few speculations: Undoped polyacetylene has a bond-charge-density-wave ground state, which implies that it is in the regime $g_1^T, g_c^T < 0$, and $g_3^T > 0$, although it is probably not true that the electron-electron interactions are strong compared to the electron-phonon interactions. (For our purposes, this is a minor point.) For doping concentration x between 1% and 5%, polyacetylene has been observed to have a reasonably high, roughly temperature-independent conductivity, but vanishingly small Pauli susceptibility,[14] suggesting spinless charge carriers. The solitons are known[15] to have effective mass $m^* \approx 3m_e$, so that for x between 0.01 and 0.05, the degeneracy energy $E^* = [(\hbar\pi)^2/2m^*](x/a)^2$ varies from 25 to 700 K. Thus, there is the intriguing possibility that moderately doped polyacetylene is in the SR-RVB-like state we have characterized, and is prevented from being a high-temperature superconductor only by the high degree of disorder in currently available materials, or by the weakness of the Josephson coupling between chains.

We acknowledge important discussions with V. J. Emergy, D. H. Lee, D. S. Rokhsar, and A. J. Heeger. This work was supported in part by National Science Foundation Grant No. NSF-DMR 83-18051.

---

[a]On leave from Central Research Institute for Physics, Budapest, Hungary.

[1a]For reviews, see J. Solyom, Adv. Phys. **28**, 201 (1979); V. J. Emery, in *Highly Conducting One Dimensional Solids,* edited by J. T. Devreese, R. Evrard, and V. Van Doren (Plenum, New York, 1979), p. 247.

[1b]Yu. A. Firsov, V. N. Prigodin, and Ch. Seidel, Phys. Rep. **126**, 245 (1985).

[2]W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).

[3]T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959).

[4]L. G. Caron and C. Bourbonnais, Phys. Rev. B **29**, 4230 (1984).

[5]G. S. Grest *et al.*, Phys. Rev. B **14**, 1225 (1976).

[6]W.-K. Wu and S. Kivelson, Phys. Rev. B **33**, 8546 (1986).

[7]S. Kivelson, A. J. Luther, and G. T. Zimanyi, unpublished.

[8]A. Luther and V. J. Emery, Phys. Rev. Lett. **33**, 589 (1974).

[9]P. Fazekas and P. W. Anderson, Philos. Mag. **30**, 432 (1974).

[10]S. Kivelson, D. Rokhsar, and J. Sethna, Phys. Rev. B **35**, 8865 (1987).

[11]P. W. Anderson, Science **235**, 1196 (1987); G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987).

[12]V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987).

[13]S. Kivelson and G. T. Zimanyi, to be published.

[14]T. C. Chung, F. Morases, J. D. Flood, and A. J. Heeger, Phys. Rev. B **29**, 2341 (1984).

[15]Z. Vardeny, J. Ornstein, and G. L. Baker, J. Phys. (Paris), Colloq. **44**, C3-329 (1983).