Solvable Two-Band Model of Fermions

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A two-band model of spinless fermions in one dimension is constructed. Density-density couplings, umklapp scattering, and interband transitions are included. Renormalization-group equations are derived and discussed. In addition, it is shown that with one condition on the couplings and the velocities the model may be transformed to two uncoupled sine-Gordon Hamiltonians, which makes it possible to obtain solutions in regions where the renormalization-group equations are not valid. An important property of the model is that there can be superconductivity with repulsive interactions.

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There are several problems of current interest for which it is necessary to study a two-band model of electrons in a solid: fluctuating-valence compounds, organic superconductors, and heavy-electron superconductors. In this Letter we shall consider a two-band model of spinless fermions in one dimension as a first step towards a general theory. Such a model simplifies the problem in such a way that it retains much of the essential physics and yet it is possible to carry out a fairly complete analysis of its behavior. It will be shown that with one condition on the coupling constants and Fermi velocities, the system may be reduced to two independent sine-Gordon Hamiltonians and is, therefore, soluble. The separability condition cannot be satisfied in weak coupling, and so is not evident in a conventional fermion renormalization-group treatment. An important property of the model is that there can be superconductivity with repulsive interactions.

A one-dimensional model of valence-fluctuation materials has been introduced by Varma and Zawadowski,[1] who derived renormalization-group equations analogous to those of the single-band electron gas in one dimension.[2] In the simplest situation, there were six coupled equations which were solved numerically in a limited regime appropriate for the valence fluctuation problem. It is clearly desirable to have a more complete discussion of this model particularly because physically interesting regions with qualitatively new physical properties may involve scaling towards strong coupling where the renormalization-group equations are not valid.

In the case of organic conductors, it is usual to consider single-band models[2] on the grounds that there is just one important spatial state for an electron or hole on the constituent organic molecules. However, it has been pointed out[3] that, for organic *superconductors,* the excitation energy to the next level is not negligible in comparison to the transfer integral so that the possibility of a second band should be taken into account. The model to be studied assumes that the bands overlap, which is consistent with one of the band structures[4] proposed for organic superconductors. The model is one dimensional, which is appropriate above a crossover temperature estimated[3] to be between 10 and 80 K. An essential feature of organic superconductors is that umklapp scattering from the anion lattice is "screened" by electron-electron correlations at all temperatures.[5] This requirement is supported by the recent discovery[6] of a structural phase transition which enhances umklapp scattering without diminishing the conductivity. For a single band this in turn implies[5] an attractive interaction between electrons on the same organic stack which is sufficiently strong to overcome the Coulomb repulsion. But this is not easy to reconcile with the known properties of organic conductors in general.[3] It will be seen that a two-band model provides an alternative and more plausible mechanism for the irrelevancy of umklapp scattering.

We shall make the simplification of omitting the spin of the electrons. In the case of the organic superconductors this is justified because the couplings which appear in the spin degrees of freedom are irrelevant variables, and the physics is governed by the charge-density waves.[5] It is also appropriate in the limit of strong repulsive on-site interactions, where the role of spin is suppressed.[2] Since the general problem is quite complicated,[1] it is useful to start out with a study of the spinless case, which has fewer degrees of freedom.

The model we consider is a natural extension of the Luttinger model in which the fermions have an internal degree of freedom σ. In the present case σ is the band index ($\sigma = a,b$) whereas in the usual theory of the one-dimensional electron gas[2] it is the spin. The

new features of the two-band model are that the Fermi velocities v_a, v_b and wave vectors k_a, k_b are unequal, and that the interactions are not invariant under rotations in σ space. The major consequence of this is that, in general, the decoupling of the "charge"-density and "spin"-density degrees of freedom, which is an essential element in obtaining exact solutions,[2] no longer holds true.

As usual, the interaction terms are two types. The first may be written in terms of the densities $\rho_{l\sigma}$ and also occur in the Luttinger model:

$$H_1' = \sum_{\sigma,\sigma'=a,b} g_{\sigma\sigma'}\rho_{1\sigma}\rho_{2\sigma'}. \tag{1}$$

Here, $\rho_{i\sigma} = \psi_{i\sigma}^\dagger \psi_{i\sigma}$ where $\psi_{i\sigma}$ annihilates fermions with band index σ moving to the right ($\psi_{1\sigma}$) or the left ($\psi_{2\sigma}$). The couplings g_{aa}, g_{bb} and $g_{ab} = g_{ba}$ are different in general, but in the symmetric limit they are related to the usual backward and forward scattering processes, g_1 and g_2,[2] by $g_{aa} = g_{bb} = g_2 - g_1$ and $g_{ab} = g_2$. Terms of the form $\rho_{i\sigma}\rho_{i\sigma}$ may be absorbed in the Fermi velocities. A $\rho_{ia}\rho_{ib}$ coupling could be taken into account but it will be omitted from the present discussion because it complicates the renormalization-group equations without changing the essential physics.

The second type of interaction consists of umklapp scattering and interband transitions:

$$H_2' = g_3(\psi_{2a}^\dagger\psi_{2b}^\dagger\psi_{1b}\psi_{1a} + \text{H.c.}) + g_f(\psi_{2a}^\dagger\psi_{1a}^\dagger\psi_{1b}\psi_{2b} + \text{H.c.}). \tag{2}$$

The umklapp term g_3 is important if there is a "joint" half-filled band such that $2(k_a + k_b)$ is equal to a reciprocal lattice vector, as in the organic superconductors.[5] Backward scattering involving $\psi_{2a}^\dagger\psi_{1b}^\dagger\psi_{2b}\psi_{1a}$ is omitted because it is important when k_a is much different from k_b. The significant new element is the interband-scattering term with coupling constant g_f. Such an interaction does not occur in the Fermi gas with spin unless there is a spin-orbit coupling,[7] and even then it is quite weak.

In order to obtain a complete picture of the properties of a one-dimensional model, it is necessary to use both the renormalization-group method and boson representations.[2] Following the standard derivations,[2] the renormalization-group equations to lowest order in the coupling constants are

$$\bar{g}_{aa}' = \tfrac{1}{2}\gamma(\bar{g}_3^2 - \bar{g}_f^2), \tag{3a}$$

$$\bar{g}_{bb}' = \tfrac{1}{2}\gamma(\bar{g}_3^2 - \bar{g}_f^2), \tag{3b}$$

$$\bar{g}_{ab}' = \tfrac{1}{2}(\bar{g}_3^2 + \bar{g}_f^2), \tag{3c}$$

$$\bar{g}_f' = \tfrac{1}{2}\bar{g}_f(2\bar{g}_{ab} - \bar{g}_{aa} - \bar{g}_{bb}), \tag{3d}$$

$$\bar{g}_3' = \tfrac{1}{2}\bar{g}_3(2\bar{g}_{ab} + \bar{g}_{aa} + \bar{g}_{bb}), \tag{3e}$$

where $g' = dg/dl$ (l is the logarithm of a cutoff), $\gamma = (v_a + v_b)^2/4v_a v_b$, $\bar{g}_{aa} = g_{aa}/\pi v_a$, $\bar{g}_{bb} = g_{bb}/\pi v_a$, and $\bar{g} = 2g/\pi(v_a + v_b)$ for $\bar{g} = \bar{g}_{ab}$, $\bar{g}_3$, or $\bar{g}_f$. It follows immediately from these equations that $\bar{g}_{aa} - \bar{g}_{bb}$ is an invariant and that there is a hyperplane $\bar{g}_f = \bar{g}_3 = 0$ of fixed points which are stable when $2\bar{g}_{ab} < -|\bar{g}_{aa} + \bar{g}_{bb}|$. It is also easy to show that the domain of attraction of the fixed hyperplane is

$$(2\bar{g}_{ab} + \bar{g}_{aa} + \bar{g}_{bb}) < -[(1+\gamma)/2]^{1/2}|\bar{g}_3|$$

when $\bar{g}_f = 0$ and

$$(2\bar{g}_{ab} - \bar{g}_{aa} - \bar{g}_{bb}) < -[(1+\gamma)/2]^{1/2}|\bar{g}_f|$$

when $\bar{g}_3 = 0$. Equations (3) are most useful in that domain because renormalized coupling constants remain small.

In the symmetric limit $v_a = v_b$ (or $\gamma = 1$) and $g_{aa} = g_{bb}$, Eqs. (3) are identical to the renormalization-group equations for a single band of fermions with spin (equal to a or b). In that case,[2] they reduce to two independent pairs of equations—one pair for charge-density waves (involving $\bar{g}_3$ and $2\bar{g}_{ab} + \bar{g}_{aa} + \bar{g}_{bb}$) and the other for the spin-density waves (involving $\bar{g}_f$ and $2\bar{g}_{ab} - \bar{g}_{aa} - \bar{g}_{bb}$). Not only does this separation simplify the analysis of Eqs. (3) but it also makes it possible to obtain exact solutions with the aid of boson representations of the fermion operators.[2] For the general two-band model, the charge and spin degrees of freedom are always coupled in Eqs. (3) and there is no sign of a potential simplification. However, we shall now show that this is a consequence of the assumption of small $g_{\sigma\sigma'}$: With one condition on the coupling constants and velocities, the charge- and spin-density waves are decoupled *even for distinct bands,* and the problem reduces to two independent sine-Gordon models.

To see how this comes about, we linearize the energy spectrum and introduce the boson representation of the fermion field[2]:

$$\psi_{l\sigma} = (2\pi s)^{-1/2}\exp\{-i\sqrt{\pi}[\int_{-\infty}^{x}\pi_\sigma(x')\,dx' \pm \phi_\sigma(x)] \mp ik_\sigma x\}, \tag{4}$$

where the upper signs correspond to $i = 2$, the lower signs to $i = 1$, and s is a cutoff related to the bandwidth (or lattice spacing) in a lattice model. The $\phi_\sigma(x)$ are boson fields and $\pi_\sigma(x)$ their conjugate momenta. With this representation, the full Hamiltonian, including the kinetic energy, may be expressed entirely in terms of boson

variables as[2]

$$H = H_0 + H', \tag{5}$$

$$H_0 = \frac{1}{2}\left[\boldsymbol{\pi}^T A \boldsymbol{\pi} + \left(\frac{\partial \boldsymbol{\phi}^T}{\partial x}\right) B \left(\frac{\partial \boldsymbol{\phi}}{\partial x}\right)\right], \tag{6}$$

$$H' = \frac{g_3}{(2\pi s)^2}\cos(2\pi^{1/2}\boldsymbol{\beta}^T\boldsymbol{\phi}) + \frac{g_f}{(2\pi s)^2}\cos[2\pi^{1/2}\int_{-\infty}^{x} dx' \boldsymbol{\alpha}^T \boldsymbol{\pi}(x')], \tag{7}$$

where $\boldsymbol{\pi}^T = (\pi_a, \pi_b)$, $\boldsymbol{\phi}^T = (\phi_a, \phi_b)$, $\boldsymbol{\alpha}^T = (1, -1)$, $\boldsymbol{\beta}^T = (1, 1)$, and A, B are symmetric 2×2 matrices, $A = V - G$ and $B = V + G$ such that $G = (g_{\sigma\sigma'})$, and V is diagonal with elements v_a and v_b. The superscript T denotes transpose.

Since H_0 is quadratic in boson fields it can be diagonalized by a canonical transformation. Define the new fields

$$\pi_i = \lambda_i^{-1/4}\mathbf{u}_i^T\boldsymbol{\pi}, \quad \phi_i = \lambda_i^{1/4}\mathbf{u}_i^T A^{-1}\boldsymbol{\phi}, \tag{8}$$

where λ_i and $\mathbf{u}_i$ (for $i = 1, 2$) are eigenvalues and eigenvectors of AB:

$$AB\mathbf{u}_i = \lambda_i \mathbf{u}_i. \tag{9}$$

The transformation (8) is canonical because of the orthonormality condition $\mathbf{u}_j^T A^{-1}\mathbf{u}_i = \delta_{ij}$. With this transformation, H_0 is diagonal but the total Hamiltonian has a *coupled* sine-Gordon form, because, in general, the arguments of the cosines in Eq. (7) contain both ϕ_1 and ϕ_2 or both π_1 and π_2.

We now observe that H' separates into two *uncoupled* cosine terms if $\boldsymbol{\alpha}$ is an eigenvector of AB, specifically $\boldsymbol{\alpha} \sim \mathbf{u}_2$. In that case, it is evident from Eq. (8) that the g_f term in Eq. (7) involves only π_2. But, since $\boldsymbol{\alpha}^T\boldsymbol{\beta} = 0$, it follows from the orthonormality condition that $\boldsymbol{\beta} \sim A^{-1}\mathbf{u}_1$, and hence from Eq. (8) $\boldsymbol{\beta}^T\boldsymbol{\phi} \sim \phi_1$ and the umklapp term in Eq. (7) contains only ϕ_1. As a consequence the full Hamiltonian separates into two uncoupled sine-Gordon models[8]:

$$H_1 = \tfrac{1}{2}\lambda_1^{1/2}\left[\pi_1^2 + \left(\frac{\partial\phi_1}{\partial x}\right)^2\right] + \frac{g_3}{(2\pi s)^2}\cos[(8\pi\theta_1)^{1/2}\phi_1(x)], \tag{10}$$

$$H_2 = \tfrac{1}{2}\lambda_2^{1/2}\left[\pi_2^2 + \left(\frac{\partial\phi_2}{\partial x}\right)^2\right] + \frac{g_f}{(2\pi s)^2}\cos\left[\left(\frac{8\pi}{\theta_2}\right)^{1/2}\int_{-\infty}^{x}\pi_2(x')\,dx'\right], \tag{11}$$

where

$$\theta_1 = \tfrac{1}{2}\lambda_1^{-1/2}\boldsymbol{\beta}^T A\boldsymbol{\beta}, \quad \theta_2^{-1} = \tfrac{1}{2}\lambda_2^{1/2}\boldsymbol{\alpha}^T A^{-1}\boldsymbol{\alpha}. \tag{12}$$

From the definitions below Eq. (7), α is an eigenvector of AB in the symmetric limit ($v_a = v_b$, $g_{aa} = g_{bb}$), or if

$$v - g_{ab}/2\pi = (g/2\pi)(\delta g/2\pi\delta v), \tag{13}$$

which is one condition on the three coupling constants and two Fermi velocities. Here $v = \frac{1}{2}(v_a + v_b)$, $g = \frac{1}{2}(g_{aa} + g_{bb})$, $\delta v = v_a - v_b$, and $\delta g = g_{aa} - g_{bb}$.

The properties of the sine-Gordon equation are sufficiently well known that reduction to Eqs. (10) and (11) constitute a "solution" of the model but, if required, there is sufficient freedom to choose $\theta_1 = \frac{1}{2}$ and $\theta_2 = 2$ to obtain the free-Fermion limit[2] for which calculations may easily be carried out. For small g_3 and g_f, there is a soliton gap for the ϕ_1 modes when $\theta_1 \lesssim 1$ and for the ϕ_2 modes when $\theta_2 \gtrsim 1$.

The presence of these gaps allows us to evaluate the various correlation functions for temperature T much larger or much smaller than the gap Δ. When $T >> \Delta$, the umklapp-scattering and the interband-transition contributions to H_i may be ignored and the correlation function χ may be evaluated in the standard way.[2] They have power-law behavior, $\chi \sim \omega^{\mu}$. The major differences from the symmetric case come from the fact that $\phi_1 \sim \phi_a + \phi_b$ and $\pi_2 \sim \pi_a - \pi_b$ are "isocharge"- and "isospin"-density operators, but their conjugate variables are not [see Eq. (8)]. One consequence is that the exponents μ are in general different for the two types of fermions. A full discussion will be presented in a future publication.

The low-temperature properties are significantly affected by the existence of an energy gap. For the present we shall take $g_3 = 0$ and only sketch the results for the more interesting case where g_f is relevant so that $\theta_2 > 1$. Then there is a gap in the ϕ_2 mode, which removes the power-law singularities in the "charge-density-wave" correlation functions as well as for pairing between two different types of fermions. Using the high-temperature exponents when the isospin degrees of freedom are frozen, we find that the superconducting correlation (SC) involving the same type of fermions has the dominant divergence for $\theta_1 > 1$, while the "isospin-density wave" (ISDW) is favored for $\theta_1 < 1$. For the symmetric case, the condition $\theta_1 > 1$ for SC implies $g + g_{ab} < 0$, i.e., attractive in-

teraction between fermions. For the asymmetric case, the condition written in terms of the couplings and velocities is

$$2\frac{g+g_{ab}}{2\pi}\left[v-\frac{g+g_{ab}}{2\pi}\right]<\left(\frac{\delta v}{2}\right)^2\left[\left(\frac{\delta g}{2\pi\delta v}\right)^2-1\right],$$

with $v>(g+g_{ab})/2\pi$. Thus for $\delta g/2\pi\delta v>1$, it is possible to satisfy the inequality with $g+g_{ab}>0$. In other words, one can get superconductivity out of entirely repulsive interactions.[9]

The separability condition (13) cannot be satisfied for weak coupling, except in the symmetric limit. Therefore, it is not surprising that the possibility of a decoupling into two sine-Gordon equations is not evident in the renormalization-group equations (3), since the right-hand sides of these equations are the leading terms of expansion in powers of $g_{\sigma\sigma'}$. The renormalization-group equations for the full sine-Gordon Hamiltonian, (5)–(7), do not require such an expansion but only assume that $|g_f|$ and $|g_3|$ are small.[2] Two of these equations give the anomalous dimension of g_f and g_3. For small $g_{\sigma\sigma'}$, they reduce to Eqs. (3d) and (3e), but for intermediate coupling when Eq. (13) is satisfied they agree with the corresponding equations obtained from (10) and (11) separately in the continuum limit $g_3\rightarrow 0$ and $g_f\rightarrow 0$.

We have applied the same approach to a two-band model of fermions with spin. Then there are four collective modes and the Hamiltonian cannot be separated if all important interactions are included. However, it is still possible to make progress if the remaining couplings are irrelevant variables. The method may also be applied to fermions with a nonlinear coupling to phonons, which is another problem involving different velocities. These questions will be considered in a future publication.

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