Superconducting Fluctuations in a Multi-Band 1D Hubbard Model

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Abstract

A renormalization-group and bosonization approach for a multi-band Hubbard Hamiltonian in one dimension is described. Based on the limit of many bands, it is argued that this Hamiltonian with bare repulsive electron-electron interactions is scaled under specific conditions to a model in which superconducting fluctuations dominate.

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The Hubbard model plays a paradigmatic role in understanding many-body correlation effects. Stimulated by the discovery of high-$T_c$ superconductivity, it has been subject of renewed interest and its multi-band versions with purely repulsive interactions have been examined as possible realizations of superconductivity [1]. However, the first study of multi-band Hubbard models date back to Van Vleck [2] who evoked intra-atomic interactions between orbitally degenerate states as an explanation for ferromagnetism. In general, these models are fascinating because, due to orbital degeneracy, they incorporate a variety of intriguing physical phenomena, including, for example, the coexistence of orbital superlattice and magnetic orderings [3]. One potential application of multi-band models could be doped fullerenes — e.g., $C_{60}$ with three- and five-fold degenerate $t_{1u}$ and $h_u$ bands — where the consequences of band degeneracy are certainly important in understanding the physics of these novel materials.

While the above studies mostly consider narrow bands or only a few degenerate bands within mean-field approximation, Muttalib and Emery [4] studied recently a two-band model of spinless electrons in one dimension by abelian bosonization and renormalization-group analysis. Interestingly, they found that superconductivity can exist with repulsive electron-electron interactions. They also considered the question of decoupling of dynamical degrees of freedom which they found to occur only at some specific values of coupling constants.

Motivated by the above examples, we focus in this paper on a novel, degenerate multi-band Hubbard model for fermions with spin degrees of freedom. We first derive one-loop renormalization-group equations and analyze their behaviour. Solvable limits of this model are then studied by bosonization. We argue that, for a particular choice of parameters, the model exhibits enhanced superconducting fluctuations. We conclude by noting that the decoupling of dynamical degrees of freedom does not occur in general, in contrast to the one-band Hubbard model.

Specifically, our starting point is the Hamiltonian

$$H = -t \sum_{n\alpha\sigma} (c_{n+1\alpha\sigma}^\dagger c_{n\alpha\sigma} + h.c.) + \frac{1}{2} \sum_{n\alpha\beta} U_{\alpha\beta} \rho_{n\alpha} \rho_{n\beta},$$  

(1)
where $c_{n\sigma}$ is the fermion operator for an electron of spin $\sigma$ with band index $\alpha$ and $\rho_{n\alpha} = \sum_{\sigma} c_{n\alpha\sigma}^\dagger c_{n\alpha\sigma}$ at site $n$. We associate the band degeneracy to colour degrees of freedom and spin degeneracy to flavour degrees of freedom; the corresponding indices take values $\alpha = 1, \ldots, N_C$ and $\sigma = 1, \ldots, N_F$. $U_{\alpha\beta}$ is the on-site electron-electron interaction which takes into account possible couplings between various bands, and $t$ is the hopping amplitude which has been assumed to be the same for all the bands. In the absence of electron-electron interactions, the model has the $U(N_C \times N_F)$ symmetry which is preserved for $U_{\alpha\beta} \equiv U$. By including more than one band and allowing the broken colour symmetry, interesting possibilities arise, one of which is enhanced superconducting fluctuations, as seen below. In the following, we always assume the full spin-rotational symmetry.

Our primary results can be qualitatively explained by considering the Hubbard interaction in the $U(N_F)$-invariant form of

$$\frac{1}{2} U_\perp \sum_n \left( \sum_\alpha \rho_{n\alpha} \right)^2 + \frac{1}{2} (U_\parallel - U_\perp) \sum_{n\alpha} \rho_{n\alpha} \rho_{n\alpha},$$

where we have assumed that the diagonal interactions can be parametrized by $U_\parallel$ and the off-diagonal interactions by $U_\perp$. Subsequently, we will be mostly interested in cases where $U_\perp \geq 0$ while $U_\parallel$ may have an arbitrary sign. Our results are: (i) In the limit of $N_C \to \infty$, $U_\perp$ scales to zero while $U_\parallel - U_\perp$ is invariant under the scaling. Thus, the model will scale to $N_C$ independent systems whose on-site electron-electron interactions are either attractive or repulsive, depending on the sign of $U_\parallel - U_\perp$. This is expected, because the mean-field approach should work in this limit and so the first term in Eq. (2) is qualitatively unimportant. (ii) For finite but large $N_C$, the system again scales so that $U_\perp$ decreases and renormalized diagonal interaction may be positive or negative. However, if initially $U_\parallel < U_\perp$, there exists a limiting value for the effective $U_\perp$ after which further scaling causes it to increase. This critical value scales as $1/N_C$. **Current Algebra and the Action.** We will use the current-algebra formalism in the calculations because it provides a compact notation and allows operator-product expansions to be used efficiently in deriving the scaling equations as short-distance degrees of freedom are
integrated out. Since we are interested in low-energy and long-wavelength phenomena, the spectrum is linearized at the Fermi energy and the fermionic degrees of freedom are expressed by slowly varying fields $\psi_{\alpha\sigma}(x\pm)$, where the left (+) and right (−) moving electrons are labeled according to their arguments, $x\pm = t \pm x$. We define $J_{\alpha\alpha'}^{\sigma\sigma'}(x\pm) = :\psi_{\alpha\sigma}^\dagger(x\pm)\psi_{\alpha'\sigma'}(x\pm):$ which present the left and right moving currents; the upper (lower) indices of the current refer to the flavour (colour) degrees of freedom. The colons denote normal orderings with respect to the filled Fermi sea of the noninteracting system. Flavour and colour currents are then defined naturally as $J^a(x\pm) = \tau^a_{\sigma\sigma'}J^{\sigma\sigma'}_{\alpha\alpha'}(x\pm)$ and $J^A(x\pm) = T^A_{\alpha\alpha'}J^{\sigma\sigma'}_{\alpha\alpha'}(x\pm)$, respectively (hereafter a sum over repeated indices is implied). Hermitian matrices $\tau^a$ and $T^A$ form a Lie algebra of SU($N_F$) and SU($N_C$) groups. Note that it is convenient to add the identity matrix to the above sets of generators; for example $\tau^0 = 1/\sqrt{N_F}$. Therefore, both currents actually give the U(1) current with $a = A = 0$, whereas $J^a$ and $J^A$ are the true SU($N_F$) and SU($N_C$) currents for nonzero $a$ and $A$. It is easy to compute the current commutation relations, equivalent to the Kac-Moody algebra. However, more useful is the corresponding operator-product expansion,

$$J_{\alpha\alpha'}^{\sigma\sigma'}(z\pm)J^{\mu\mu'}_{\beta\beta'}(w\pm) = \pm \frac{\delta_{\alpha\beta}\delta_{\alpha'\beta'}\delta_{\mu\mu'}\delta_{\sigma\sigma'}}{4\pi^2(z\pm - w\pm)^2}$$

$$+ \frac{J_{\alpha\beta}(z\pm)\delta_{\alpha'\beta'}\delta_{\sigma\mu'} - J_{\beta'\alpha'}^{\mu\mu'}(z\pm)\delta_{\alpha\beta}\delta_{\sigma\mu}}{2\pi(z\pm - w\pm)} + \cdots.$$  

This follows from the commutator and can be shown by means of the conformal symmetry. Here we assume radial quantization where the spatial dimension is compactified by mapping the space and time coordinates to a cylinder of radius $2\pi; z\pm = \exp(t \pm ix)$. Below, we continue to use the flat space-time coordinates for the action but do the actual calculations in the complex plane.

The free part of the action is

$$S_o = \frac{\pi}{N_C + N_F} \sum_{s = \pm} \int d^2x [J^a(x_s)J^a(x_s) + J^A(x_s)J^A(x_s)],$$

and the action describing the electron-electron interaction is
where $d^2x = dx dt$ and the units are defined so that the Fermi velocity becomes $\hbar v_F = 1$. In contrast to the Hubbard model, we will allow the coupling constants $U^{(k)}$ to be independent, as implied by various physically important interactions — for example, by the nearest-neighbour electron-electron interaction.

**Renormalization-Group Equations and the Flow.** We follow the usual procedure in which the partition function, $Z = \int \mathcal{D}[\psi] e^{-S}$, is regularized by introducing a ultraviolet cutoff $\ell$ for short distances. As the short-distance degrees of freedom are integrated out continuously by using the operator-product expansion \([3]\), the coupling constants are correspondingly renormalized so that $Z$ remains unchanged \([1,2]\). This procedure then gives the one-loop scaling equations for the coupling constants:

$$
\frac{\partial}{\partial \ell} g_{\parallel} = -(g_{\parallel}^2 + g_{\perp}^2) + [(g_{\parallel}^2 + g_{\perp}^2) - g_{\parallel}^2]/NC
$$

$$
\frac{\partial}{\partial \ell} g_{\perp} = -(g_{\parallel}^2 + g_{\perp}^2) + [(g_{\parallel} - 2g_{\parallel}) - g_{\perp} + 2g_{\perp}]g_{\perp} + (2g_{\perp} - g_{\parallel})g_{3\perp}]/NC
$$

$$
\frac{\partial}{\partial \ell} g_{\parallel2} = (g_{3\parallel} - g_{\parallel1}^2)/2NC
$$

$$
\frac{\partial}{\partial \ell} g_{\perp2} = (g_{3\perp} - g_{\perp1}^2)/2NC
$$

$$
\frac{\partial}{\partial \ell} g_{3\parallel} = -2g_{1\perp}g_{3\perp} + [(2g_{\parallel} - g_{\parallel1})g_{3\parallel} + 2g_{1\perp}g_{3\perp}]/NC
$$

$$
\frac{\partial}{\partial \ell} g_{3\perp} = -2g_{1\perp}g_{3\perp} + [(g_{\parallel} + g_{\perp1} - 2g_{\parallel} + 4g_{1\perp})g_{3\perp} - g_{3\parallel}g_{1\perp}]/NC,
$$

where $g_{k\parallel,\perp} = NCU^{(k)}_{\parallel,\perp}/\pi$ ($k = 1, \ldots, 4$) and $N_F = 2$ is chosen. The coupling constants are functions of the ultraviolet cutoff $\ell$; $\partial / \partial \log \ell$. As usual, $g_{1\alpha}$ is the backward-scattering constant, $g_{2\alpha}$ is the forward-scattering constant, and $g_{3\alpha}$ is the Umklapp-scattering constant ($\alpha = ||, \perp$). Because $g_{3\alpha}$ corresponds to the scattering processes which violate momentum conservation by $4k_F$, it is important only if $4k_F$ is equal to the reciprocal lattice constant; $k_F$ is the Fermi wavevector which has been assumed to be the same for all the bands. We have ignored $g_{4\alpha}$ because its only effect is to renormalize Fermi velocities; although this could be taken into account, $g_{4\alpha}$ does not enter at one-loop order since $\int dz/z^2 = 0$. 


Because the parameter space of the system is very large, we have investigated the scaling behaviour of the system in two special cases:

(1) First, we consider the system with the broken orbital $U(N_C)$ symmetry so that the action is only $U(N_F)$ invariant. We further set the forward-scattering coupling temporally to zero, $g_{2\parallel,\perp} = 0$, because the backward- and Umklapp-scattering coupling constants are the most relevant ones in terms of that their scaling behaviour is nontrivial. By letting initially $g_{\parallel,\perp} = g_k\parallel,\perp$ ($k = 1, 3$), and $g_{2\parallel,\perp} = 0$, these properties are conserved by the renormalization-group flow. Thus,

$$\begin{align*}
\partial_t g_{\parallel} &= -2g_{\perp}^2 + (2g_{\perp}^2 - g_{\parallel}^2)/N_C, \\
\partial_t g_{\perp} &= -2g_{\perp}^2 + (4g_{\perp}^2 - 3g_{\parallel}^2)g_{\perp}/N_C;
\end{align*}$$

with $N_F = 2$. It is easy to see from these equations that the renormalization-group flow may change the sign of $g_{\parallel}$ but not the sign of $g_{\perp}$. In fact, $g_{\perp} = 0$ forms a fixed point for this coupling constant. This, and the line $g_{\perp} = g_{\parallel}$ act as separatrices: (i) First, let $g_{\perp} > g_{\parallel} \geq 0$. Now there is also another relevant solution for the equation $\partial_t g_{\perp} = 0$: $g_{\perp} = -3g_{\parallel}/(2N_C - 4)$. This solution yields a turning point for the scaling trajectories at which the initially decreasing $g_{\perp}$ starts to increase. For large $N_C$, the turning value of $g_{\perp}$ scales as $1/N_C$. Note that $g_{\parallel}$ decreases monotonically and, at the turning point, $g_{\parallel} < 0$. (ii) In the region $g_{\parallel} \geq g_{\perp} \geq 0$, the system scales towards a noninteracting model ($g_{\parallel,\perp} = 0$), corresponding to the $N_C$ free fermion theories. (iii) Finally, $g_{\perp} < 0$ leads always to the strongly attractive interactions: $g_{\parallel}$ and $g_{\perp}$ decrease without bound at one-loop order.

To illustrate the general behaviour of Eqs. (7), we integrate them numerically and plot the renormalization-group flow for $N_C = 10$; see Fig. 1. For $g_{\perp} > g_{\parallel} > 0$, it clearly shows the tendency of the renormalization-group flow to lead to an effective Hamiltonian which contains weakly coupled one-band Hamiltonians with intraband electron-electron attractions. It is then convenient to diagonalize each of these Hamiltonians separately and to take into account the off-diagonal interactions perturbatively. However, this assumption relies on the fact that the “unperturbed” system has a gap the perturbation expansion to work. These results apply to Eqs. (3) whose qualitative behaviour is similar for finite $g_{2\parallel,\perp}$.
We next consider the model with the full \( U(N_C \times 2) \) symmetry: \( U^{(k)}_{\alpha\beta} = U^{(k)}, \ k = 1, \ldots, 4 \). In this case, the interaction term becomes

\[
S_I = \int d^2x \left( -U^{(1)} J^{A_A}(x_+) J^{A_A}(x_-) + U^{(2)} J(x_+) J(x_-) + \frac{1}{2} U^{(4)} [J(x_+) J(x_+) + J(x_-) J(x_-)] + \text{Umklapp} \right),
\]

where \( J^{A_A}(x_\pm) = \tau^a_{\sigma\sigma'} T^{A_A}_{\alpha\alpha'}(x_\pm) \) is the colour-flavour current and \( J \equiv J^{00} \) is the \( U(1) \) current. As an example, we assume that the bare interactions are repulsive \((g_k > 0)\). In this case and at half filling, \( g_1 \) can scale to large negative values, \( g_2 \) is renormalized only weakly, and \( g_3 \) decreases and starts to increase approximately when \( g_1 \) becomes negative. Note that the renormalized value of \( g_3 \) is always positive. It is very difficult to draw any conclusions, even at \( g_1 = 0 \) for \( g_3 \neq 0 \) (the half-filled case), although the interesting feature is that the backward-scattering coupling constant \( g_1 \) scales towards large negative values which may suggest enhanced density-wave fluctuations in colour or flavour channel. In general, an analytical solution does not seem to be possible when \( g_1 \) and \( g_3 \) are the most dominant coupling constants.

**Bosonization.** We now turn to a limit where the backward and Umklapp terms are either zero or scale to zero, so that the multi-band model is exactly solvable by bosonization \[^8]^9\]. In particular, we consider the \( U(N_F) \)-invariant model where the \( U(N_C) \) symmetry is broken by letting \( U_{\parallel} \neq U_{\perp} \). For our purposes, abelian bosonization \[^9\] is sufficient. At zero temperature, the most dominant instabilities are either \( 2k_F \) density-wave (DW) or superconducting (SC) instabilities whose correlation functions \[^10\] have power-law singularities at low energies and small momenta with exponents

\[
\mu_{\text{DW}} = 2(1 - \delta \theta)/N_F + 2(\delta \theta - \bar{\theta})/N_C N_F, \quad (9a)
\]

\[
\mu_{\text{SC}} = 2(1 - 1/\delta \theta)/N_F + 2(1/\delta \theta - 1/\bar{\theta})/N_C N_F, \quad (9b)
\]

where \( \delta \theta^2 = (1 + \delta u_4 - \delta u_2)/(1 + \delta u_4 + \delta u_2) \) and \( \bar{\theta}^2 = (1 + \bar{u}_4 - \bar{u}_2)/(1 + \bar{u}_4 + \bar{u}_2) \). We have defined \( \delta u_k = N_F (U^{(k)}_{\parallel} - U^{(k)}_{\perp})/4\pi \) and \( \bar{u}_k = N_F [U^{(k)}_{\parallel} + (N_C - 1) U^{(k)}_{\perp}]/4\pi \), \((k = 2, 4)\).
In these expressions, \( U^{(k)}_{\parallel,\perp} \) are the renormalized values of the forward-scattering constants. Clearly density-wave fluctuations always dominate over superconducting fluctuations for \( U^{(k)}_{\parallel} = U^{(k)}_{\perp} > 0 \) and vice versa. However, if \( 0 \leq U^{(2)}_{\parallel} < U^{(2)}_{\perp} \), superconducting fluctuations win, provided that \( N_C > (\delta \theta / \bar{\theta} - 1) / (\delta \theta - 1) \) and \( U^{(2)}_{\perp} \leq U^{(4)}_{\perp} \), where the latter condition is needed to guarantee a sensible large-\( N_C \) limit.

In contrast, if the large-\( N_C \) limit is taken so that \( g_{k\parallel,\perp} \equiv N_C N_F U^{(k)}_{\parallel,\perp} / 2\pi \) are kept constant, the condition, \( 0 \leq g_{2\parallel} < g_{2\perp} \), is no longer sufficient to have diverging superconducting correlation functions at low energies and small momenta. As an example, let \( g_{\|,\perp} = g_{k\|,\perp} \) \((k = 2, 4)\) and consider the weak-coupling limit: \( g_{\|,\perp} \ll 1 \). We find that the superconducting correlation functions are the most singular ones for the repulsive interactions and \( N_C \gg 1 \), if the condition \( g_{\|} < g_{\perp}^2 / 2 + \mathcal{O}(g_{\perp}^3) \) is satisfied \([11]\).

It is interesting to note the connection between the above consideration and the renormalization-group approach in the case of the repulsive interactions: they both imply that the necessary condition for superconducting fluctuations to dominate is \( U_{\|} < U_{\perp} \) and \( N_C \) to be large enough.

**Colour-Flavour Separation.** The scaling equations show no apparent separation into independent sectors. This not so surprising if we consider the model with the \( U(N_C \times N_F) \) symmetry. This coupling of the colour and flavour degrees of freedom — a manifestation of the fact that the colour and flavour currents are not independent dynamical variables — follows because the colour-flavour current commutes neither with the colour nor with the flavour current \([12]\). However, away from half filling, the \( U(1) \) current describes an independent dynamical degree of freedom; \( J \) commutes with the other currents. The coefficient multiplying the \( JJ \) term in Eq. (8) is \( U^{(c)} = U^{(2)} - U^{(1)} / N_C N_F \). Consequently, in the one-loop renormalization-group equations \([8]\), \( g_c \equiv N_C N_F U^{(c)} / 2\pi \) is indeed decoupled from the other degrees of freedom. Moreover, it is a scaling invariant. In the one-band Hubbard model, the spin-charge separation is evident even at half-filling, because the Umklapp term is a chiral \( SU(N_F) \) singlet \([13]\).
Relation to the Muttalib-Emery Approach \[4\]. Our approach differs in two respects from that of Ref. \[4\]: we consider an arbitrary number of bands with the spin degrees of freedom but ignore the interband Umklapp scattering. The interband Umklapp scattering would allow versatile possibilities; for example, one could include terms such as

\[ U^{(5)}_{\alpha\beta} \int d^2 x J^\alpha_{\alpha\beta}(x_+) J^\beta_{\alpha\beta}(x_-). \]

Since the scaling equations have to be invariant under the phase transformation \( \psi_{\alpha\sigma} \rightarrow e^{i\theta_{\alpha\sigma}} \psi_{\alpha\sigma}, \) \( U^{(5)}_{\alpha\beta} = 0 \) is a fixed point and the other scaling equations contain only even powers of \( U^{(5)}_{\alpha\beta} \). The question remains whether these coupling constants are (marginally) relevant. Because they do not originally appear in the Hubbard model, we have assumed that their bare values are negligible and that they do not change the scaling behaviour qualitatively. On the other hand, in the model considered in Ref. \[4\], they were found to be important. Our motivation was to illustrate that even the Hubbard model can show enhanced superconducting fluctuations if the spin and multiple bands are assumed.

Conclusion. We have shown that the existence of multiple bands can lead to enhanced superconducting fluctuations. Based on the one-loop renormalization-group analysis, we found that the renormalized diagonal electron-electron interactions are attractive and the off-diagonal electron-electron interactions are of order \( O \left( \frac{1}{N_C} \right) \), if bare values of the coupling constants are such that \( U_\parallel < U_\perp \). This is consistent with the result obtained by studying the Hamiltonian in the exactly solvable limit.

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[5] The SU($N_F$) generators are renormalized so that $\text{Tr} \, \tau^a \tau^b = \delta^{ab}$ ($a, b = 0, \ldots, N^2_F - 1$). Other useful relations are $[\tau^a, \tau^b] = i f^{abc} \tau^c$, and $\tau^a_{\sigma \sigma'} \tau^a_{\mu \mu'} = \delta_{\sigma \mu} \delta_{\sigma' \mu'}$. Note that $\tau^0 = 1/\sqrt{N_F}$. Similar equations hold for the SU($N_C$) generators $T^A$ ($A = 0, \ldots, N^2_C - 1$), where the structure factors are now denoted by $f^{ABC}$.

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[8] For the chiral U($N_C \times N_F$)-symmetric case, non-abelian bosonization is the most natural way to proceed because it has manifestly the same symmetry group as the fermionic theory. In this case, various correlation functions are easily calculated because the scaling dimensions of the fields are known. See, for example, E. Witten, Commun. Math. Phys. 92, 455 (1984); V. Knizhnik and A. Zamolodchikov, Nucl. Phys. B 247, 83 (1984); Y. Frishman and J. Sonnenschein, Nucl. Phys. B 294, 801 (1987).

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These correlation functions, which are the most singular for the present U(N_F)-invariant model, are described either by the operators $A_{FSC}^a(x, t) = \psi^{\alpha\sigma}(x_+) r^a_{\sigma\mu} \psi^{\alpha\mu}(x_-)$ (flavour-superconducting) or by $A_{SDW}(x, t) = \psi^\dagger_{\alpha\sigma}(x_+ \psi^{\alpha\sigma}(x_-)$ (scalar-density-wave) and $A_{FDW}^a(x, t) = \psi^\dagger_{\alpha\sigma}(x_+) r^a_{\sigma\mu} \psi^{\alpha\mu}(x_-)$ (flavour-density-wave) ($a \neq 0$). For the U(N_C × N_F)-invariant model, we have also other, equally divergent correlations functions at low energies, as determined by the U(N_C × N_F) generators. (If $N_C N_F \neq 2$, the operator for scalar-superconducting fluctuations is more involved and it is not considered here.) At zero momenta (relative to $2k_F$), the low-energy behaviour of the correlation functions is described by the form of $\omega^{-\mu}$ which also defines the corresponding exponent $\mu$.

If the weak-coupling limit is relaxed, this condition will become $g_{\parallel} < g_{\perp} + 2 - 2\sqrt{1 + g_{\perp}}$. Note that $\mu_{DW, SC} = O(N_C^{-1})$, for $N_C \gg 1$ and fixed $g$'s.

For example, $[J^a(x_\pm), J^{B}(y_\pm)] = if^{abc} J^{cB}(x_\pm) \delta(x_\pm - y_\pm) \pm \frac{1}{2\pi} \delta^{ab} \delta^{0B} \partial_\pm \delta(x_\pm - y_\pm)$.

I.Affleck and F.Haldane, Phys. Rev. B36, 5291 (1987).
FIGURES

FIG.1 Scaling trajectories in the \((g_{∥}, g_{⊥})\)-plane for the half-filled, \(N_C\)-band Hamiltonian for \(N_C = 10\), as given by Eq. (7) \((N_F = 2)\). The equation \(g_{⊥} = -3g_{∥}/(2N_C - 4)\) is shown by a dashed line.