Phase Diagram of the Extended Hubbard Model with Correlated-Hopping Interaction

G.I. Japaridze$^1$ and A.P. Kampf

Institut für Physik, Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Germany

A one-dimensional model of interacting electrons with on-site $U$, nearest-neighbor $V$, and correlated-hopping $T^*$ interaction $T^*$ is studied at half-filling using the continuum-limit field theory approach. The ground-state phase diagram is obtained for a wide range of coupling constants. In addition to the insulating spin- and charge-density wave phases for large $U$ and $V$, respectively, we identify bond-located ordered phases corresponding to an enhanced Peierls instability in the system for $T^* > 0$, $|U - 2V| < 8T^*/\pi$ and to a staggered magnetization located on bonds between sites for $T^* < 0$, $|U - 2V| < 8T^*/\pi$. The general ground state phase diagram including insulating, metallic, and superconducting phases is discussed.

PACS numbers: 71.27.+a, 71.10.Hf, 71.10.Fd

I. INTRODUCTION

Since the discovery of high-$T_c$ superconductivity there is continuous interest in models of interacting electrons with unconventional correlation mechanisms. Among others, models with correlated-hopping (CH) interaction [1-37] are the subject of current studies. In addition to the usual interaction between electrons on the same site ($U$) and/or on nearest-neigbor (nn) sites ($V$), these models contain terms describing the modification of the electronic hopping motion by the presence of other particles. Such a term emerges rather naturally in the construction of a tight-binding Hamiltonian [2] and describes the interaction between charges located on bonds and on lattice sites (the bond-charge interaction). Generally, a model with CH interaction can naturally be viewed either as an effective model obtained after integrating out additional degrees of freedom [3,6,8,9] or as a phenomenological model.

The CH model was first proposed by Foglio and Falikov in 1979 to describe the low-energy properties of mixed valence systems [6]. In the eighties the bond-charge coupling was discussed mainly in the context of organic conductors, e.g. doped polyacetylene, to describe the interplay between Coulomb repulsion and Peierls dimerization effects [3,6,8].

The interest in models with CH interaction increased after the discovery of high-$T_c$ superconductivity. Hirsch was the first who pointed out that the CH interaction provides a mechanism for a superconducting instability [1]. Soon after, Essler, Korepin, and Schoutens proposed the integrable supersymmetric extension of the Hubbard model with a particular, strongly correlated "kinematics" and a truly superconducting ground state of the $\eta$-pairing type [22]. These results were intensively explored later in the context of superconductivity in high-$T_c$ oxides: electrons with CH interaction were studied using the BCS type mean-field approach [13,14], the field theory renormalization-group treatment [13], the exact solution for particular values of coupling constants, and by numerical techniques [16,21]. Several exactly solvable 1D models of interacting electrons with CH coupling were proposed and intensively studied [22-27]. These models with CH interaction provide us with a unique possibility to study unconventional mechanisms for Cooper pairing, metal-insulator, and insulator-superconductor transitions.

An interesting CH model with a rich ground state phase diagram has been proposed by Simon and Aligia [3]. The 1D version of the Simon-Aligia Hamiltonian reads:

$$\mathcal{H} = t_{\text{ch}} \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} (1 - \hat{\rho}_{n,\sigma}) (1 - \hat{\rho}_{n+1,\sigma})$$
$$+ t_{cd} \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} \hat{\rho}_{n,\sigma} \hat{\rho}_{n+1,\sigma}$$
$$+ t_{dd} \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} \hat{\rho}_{n,\sigma} + \hat{\rho}_{n+1,\sigma} - 2 \hat{\rho}_{n,\sigma} \hat{\rho}_{n+1,\sigma}$$
$$+ \frac{1}{2} U \sum_{n,\sigma} \hat{\rho}_{n,\sigma} \hat{\rho}_{n,\sigma} + \sum_{n} \hat{\rho}_{n} \hat{\rho}_{n+1}$$

(1)

where $\hat{\rho}_{n,\sigma} = c_{n,\sigma}^\dagger c_{n,\sigma}$, $\hat{\rho}_{n} = \sum_{\sigma} \hat{\rho}_{n,\sigma}$, and $\hat{Q}_{n,n+1,\sigma} = c_{n,\sigma}^\dagger c_{n+1,\sigma} + c_{n+1,\sigma}^\dagger c_{n,\sigma}$. The first term interchanges an electron and a hole, while the second term interchanges an electron and a doublon (doubly occupied site) between nn sites. The effect of $t_{dd}$ is to destroy a doublon in the presence of a nn hole into two electrons on nn sites, and vice versa.

It is useful to rewrite the Hamiltonian (1) in the standard way, combining the two-body and the three-body terms. As a result the Hamiltonian is rewritten as:

$$\mathcal{H} = -t \sum_{n,\sigma} (c_{n,\sigma}^\dagger c_{n+1,\sigma} + c_{n+1,\sigma}^\dagger c_{n,\sigma}) - \mu \sum_{n,\sigma} c_{n,\sigma}^\dagger c_{n,\sigma}$$
$$+ \frac{1}{2} U \sum_{n,\sigma} \hat{\rho}_{n,\sigma} \hat{\rho}_{n,\sigma} + \sum_{n} \hat{\rho}_{n} \hat{\rho}_{n+1}$$
$$+ \frac{t^*}{2} \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} (\hat{\rho}_{n,\sigma} + \hat{\rho}_{n+1,\sigma}$$
$$+ T^* \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} \hat{\rho}_{n,\sigma} \hat{\rho}_{n+1,\sigma}$$

(2)
Here \( t^* = t_{eh} - t_{dd} \) and \( T^* = 2t_{dd} - t_{eh} - t_{ed} \). There are \( N_e \) particles, \( N_0 \) sites and the band filling \( \nu = N_e/2N_0 \) is controlled by the chemical potential \( \mu \).

The 2D version of the Hamiltonian (1) has been derived by Simon and Alicki as an effective one-band model resulting from tracing out the oxygen degrees of freedom in cuprates [3]. The model was studied by analytical and numerical methods, especially in the limit of strong interactions [25, 26, 27, 28, 29]. The main attention was focused on the search for a superconducting ground state. Away from half-filling and for \( t^* \approx t \) the properties of the system are determined by the two-body CH term \((t^*)\) and in qualitative agreement with results for the standard CH model \((T^* = 0)\) [33, 34]. There is a transition into a superconducting phase for particular band-fillings and sufficiently small on-site repulsion [28, 36]. The effective interaction originating from the \( t^* \) term which appears in the continuum-limit theory, is given by \( t^* \cos(\pi \nu) \) [3]. Therefore, in the half-filled band-case the three-body term becomes crucial. For \( t^* = t \) and \( T^* < 0 \) an insulator-metal transition for sufficiently small \( U \) and \( V \) has been demonstrated [24, 25, 26]. The nature of superconducting instabilities in the metallic phase was investigated numerically and within a mean-field approach [22, 23]. Recently, also the possibility for realizing triplet superconductivity (TS) in the ground state of the model [37, 38] has not been considered in previous studies. We show the search for bond-located ordered phases [39] and the charge-density wave (CDW) phase with order parameter \( \Delta_{\text{dimer}} = (-1)^n \sum_\sigma \hat{Q}_{n,n+1,\sigma} \) (3) at half-filling was studied [34, 35].

An important feature of the CH interaction is its site-off-diagonal nature. At half-filling this provides the principal possibility for realizing bond located ordering [37, 38]. In this paper we study the model Hamiltonian (2) using the weak-coupling field-theory approach. We focus on the search for bond-located ordered phases. Such an ordering has not been considered in previous studies. We show that for \( T^* > 0 \) the three-body interaction enhances the Peierls instability in the system. Near the frustration line \( U = 2V \) of the extended \((U-V)\) Hubbard model [39], for \(|U - 2V| < 8T^*/\pi \) and \( V > -4T^*/\pi \) the long range ordered (LRO) dimerized ground state with order parameter

\[
\Delta_{\text{dimer}} = (-1)^n \sum_\sigma \hat{Q}_{n,n+1,\sigma}
\]

is realized. For \( T^* < 0 \) the bond-located spin-density-wave (bd-SDW) phase with order parameter

\[
\Delta_{\text{bd-SDW}} = (-1)^n \sum_\sigma \sigma \hat{Q}_{n,n+1,\sigma}
\]

and the the charge-density wave (CDW) phase show an identical power-law decay of the correlation functions at large distances for \(|U - 2V| < 8T^*/\pi \) and \( V > 0 \). The \( \text{bd-SDW} \) phase corresponds to a staggered magnetization located on bonds between sites.

The paper is organized as follows: In Sect. II the symmetry of the model is reviewed. In Sect. III the continuum-limit bosonized version of the model is constructed. In Sect. IV we discuss the weak-coupling phase diagram. Finally, Sect. V is devoted to a discussion and to concluding remarks on the ground state phase diagram.

II. SYMMETRIES OF THE MODEL

In the absence of the CH interaction \((t^* = T^* = 0)\) Eq. (2) is the Hamiltonian of the extended Hubbard model. The ground state phase diagram of the 1/2-filled extended Hubbard model is well studied [39–41]: the low-energy properties of the model are essentially determined by the parameter \( U - 2|V| \). The insulating ground state for \( U > 2|V| \) is dominated by spin-density wave (SDW) correlations. The line \( U = 2|V| \) corresponds to a Luttinger liquid (LL) phase. In the case of repulsive \( nn \) interaction \((V > 0)\), the \( U = 2|V| \) line corresponds to a transition from the SDW phase \((U > 2|V|)\) into an insulating LRO CDW phase for \( U < 2|V| \) [38, 41]. In the case of attractive \( nn \) interaction \((V < 0)\) the \( U = 2|V| \) line corresponds to a transition from the insulating SDW phase into a metallic phase with dominating superconducting instabilities [40].

When the CH interaction is added to the model two new aspects appear. The first is the site-off-diagonal character of the CH coupling which provides a possibility for bond-located ordering. The second is the symmetry aspect. In the general case the CH interaction violates the electron-hole symmetry [11]. This leads to an essential band-filling dependence of the phase diagram [11, 13]. Let us first consider the symmetry aspect. The three generators of the spin-\(SU(2)\) algebra

\[
S^+ = \sum_n c_{n,\uparrow}^\dagger c_{n,\downarrow}, \quad S^- = \sum_n c_{n,\downarrow}^\dagger c_{n,\uparrow}, \quad S^z = \frac{1}{2} \sum_n (c_{n,\uparrow}^\dagger c_{n,\downarrow}^\dagger - c_{n,\downarrow}^\dagger c_{n,\uparrow}),
\]

commute with the Hamiltonian (3) which shows its \( SU(2) \)-spin invariance.

The electron-hole transformation

\[
c_{n,\sigma} \rightarrow (-1)^n c_{n,\sigma}^\dagger,
\]

converts \( \mathcal{H}(t, U, V, t^*, T^*) \rightarrow \mathcal{H}(\tilde{t}, U, V, \tilde{t}^*, T^*) \) with

\[
\tilde{t} = t - 2t^* - T^*, \quad \tilde{t}^* = -t^* - T^*
\]

and therefore the Hamiltonian (3) does possess electron-hole symmetry for \( 2t^* + T^* = 0 \).

At half-filling and for \( V = 2t^* + T^* = 0 \) the model (4) is characterized by an additional important symmetry. The transformation

\[
c_{n,\uparrow} \rightarrow c_{n,\uparrow}^\dagger, \quad c_{n,\downarrow} \rightarrow (-1)^n c_{n,\downarrow}^\dagger,
\]

interchanges the charge and spin degrees of freedom and converts
\[ \mathcal{H}(t,U,T^*) \rightarrow \mathcal{H}(t,-U,T^*). \]  
(9)

Therefore, in this case, the charge sector is governed by the same \( SU(2) \) symmetry as the spin sector and the model has the \( SU(2) \otimes SU(2) \) symmetry \( \mathcal{O} \) with generators:

\[ \eta^+ = \sum_n (-1)^n c_{n,\uparrow}^\dagger c_{n,\downarrow}, \quad \eta^- = \sum_n (-1)^n c_{n,\downarrow} c_{n,\uparrow}, \]
\[ \eta^z = \sum_n \frac{1}{2} (1 - c_{n,\uparrow}^\dagger c_{n,\downarrow} + c_{n,\downarrow} c_{n,\uparrow}). \]  
(10)

For the half-filled Hubbard model the \( SU(2) \otimes SU(2) \) symmetry implies that the gapful charge and the gapless spin sectors for \( U > 0 \) are mapped by the transformation Eq. (8) into a gapful spin and a gapless charge sector for \( U < 0 \). Moreover, at \( U < 0 \) the model is characterized by the coexistence of CDW and singlet superconducting (SS) instabilities in the ground state \[42\].

Contrary to the on-site Hubbard interaction \( U \) the \( T^* \) term remains invariant with respect to the transformation Eq. (8). This immediately implies that for a given \( T^* \) and

- for \( U = 0 \) the properties of the charge and the spin sectors are identical;
- for \( U \neq 0 \) there exists a critical value of the Hubbard coupling \( U_c \) corresponding to a crossover from the \( T^* \) dominated regime into a \( U \) dominated regime.

The LL parameters of the model characterizing the gapless charge \( K_c \) and spin \( K_s \) degrees of freedom are \( K_c = K_s = 1 \).

For nonzero nn interaction \( (V \neq 0) \) the spin \( SU(2) \)-symmetry remains unchanged, while the symmetry of the charge sector is reduced to a \( U(1) \)-symmetry (conservation of charge). In this case the gapless charge sector is parametrized by a fixed-point value of the parameter \( K_c = K_c^* \) which essentially depends on the bare values of the coupling constants. This results in a different power-law decay at large distances for density-density and superconducting correlations, supporting \( CDW \) for \( V > 0 \) and superconductivity for \( V < 0 \). However, due to the \( SU(2) \)-spin symmetry the dynamical generation of a gap in the spin excitation spectrum supports SS superconductivity. In the case of a gapless spin sector both SS and TS correlations show an identical power-law decay at large distances.

**III. CONTINUUM-LIMIT THEORY AND BOSONIZATION.**

In this section we construct the continuum-limit version of the model Eq. (2) at half-filling. While this procedure has a long history and is reviewed in many places \[43\], for clarity we briefly sketch the most important points.

The field theory treatment of 1D systems of correlated electrons is based on the weak-coupling approach \[|U|, |V|, |T^*|, |T^*| \ll t \]. Assuming that the low energy physics is controlled by states near the Fermi points \( \pm k_F \) \((k_F = \pi/2a_0, \text{where } a_0 \text{ is the lattice spacing})\) we linearize the spectrum around these points and obtain two species (for each spin projection \( \sigma \)) of fermions, \( R_\sigma (n) \) and \( L_\sigma (n) \), which describe excitations with dispersion relations \( E = \pm v_F p \). Here, \( v_F = 2t a_0 \) is the Fermi velocity and the momentum \( p \) is measured from the two Fermi points. More explicitly, one decomposes the momentum expansion for the initial lattice operators into two parts centered around \( \pm k_F \) to obtain the mapping:

\[ c_{n,\sigma} \rightarrow i^n R_\sigma (n) + (-i)^n L_\sigma (n), \]  
(11)

where the fields \( R_\sigma (n) \) and \( L_\sigma (n) \) describe right-moving and left-moving particles, respectively, and are assumed to be smooth on the scale of the lattice spacing. This allows us to introduce the continuum fields \( R_\sigma (x) \) and \( L_\sigma (x) \) by

\[ R_\sigma (n) \rightarrow \sqrt{a_0} R_\sigma (x = na_0), \]
\[ L_\sigma (n) \rightarrow \sqrt{a_0} L_\sigma (x = na_0). \]  
(12)

In terms of the continuum fields the free Hamiltonian reads:

\[ H_0 = E_0 - iv_F \sum_{\sigma} \int dx [ : R_\sigma^\dagger (x) \partial_x R_\sigma : + : L_\sigma^\dagger (x) \partial_x L_\sigma : ] \]  
(13)

which is recognized as the Hamiltonian of a free massless Dirac field and the symbols \( : \) denote normal ordering with respect to the ground state of the free system.

The advantage of the linearization of the spectrum is twofold: the initial lattice problem is reformulated in terms of smooth continuum fields and – using the bosonization procedure – is mapped to the theory of two decoupled quantum sine-Gordon (SG) models describing charge and spin degrees of freedom, respectively.

In terms of the continuum fields the initial lattice operators have the form

\[ \hat{\rho}_{n,\sigma} = \frac{1}{2} \equiv : \hat{\rho}_{n,\sigma} : \]
\[ = a_0 \{ : R_\sigma^\dagger (x) R_\sigma (x) : + : L_\sigma^\dagger (x) L_\sigma (x) : \}
\[ + (-1)^n (R_\sigma^\dagger (x) L_\sigma (x) + L_\sigma^\dagger (x) R_\sigma (x)) \}, \]  
(14)
\[ = \hat{Q}_{n,n+1,\sigma} := \hat{Q}_{n,n+1,\sigma} - \frac{2}{\pi} = 2a_0 i(-1)^n (R_\sigma^\dagger (x) L_\sigma (x) - L_\sigma^\dagger (x) R_\sigma (x)). \]  
(15)

The second step is to use the standard bosonization expressions for fermionic bilinears \[44\]:

\[ - i : R_\sigma^\dagger (x) \partial_x R_\sigma : - L_\sigma^\dagger (x) \partial_x L_\sigma : \rightarrow \frac{1}{2} \{ P_\sigma^2 (x) + (\partial_x \varphi_\sigma)^2 \}, \]  
(16)
\[ R^\dagger_\sigma(x) R_\sigma(x) : + : L^\dagger_\sigma(x) L_\sigma(x) \rightarrow \frac{1}{\sqrt{\pi}} \partial_x \phi(x), \]

\[ R^\dagger_\sigma(x) R_\sigma(x) : - : L^\dagger_\sigma(x) L_\sigma(x) \rightarrow -\frac{1}{\sqrt{\pi}} P_\sigma(x), \]

\[ R^\dagger_\sigma(x) L_\sigma(x) \rightarrow -\frac{i}{\sqrt{2\pi a_0}} \exp(-i \sqrt{4\pi} \phi(x)). \]

We thereby obtain

\[ \hat{\rho}_{n,\sigma} \rightarrow a_0 \left\{ \frac{1}{\sqrt{\pi}} \partial_x \varphi(x) - (-1)^n \frac{1}{\pi a_0} \sin(\sqrt{4\pi} \varphi(x)) \right\}, \]

\[ \hat{Q}_{n,n+1,\sigma} \rightarrow (-1)^n \frac{2}{\pi} \cos(\sqrt{4\pi} \varphi(x)), \]

\[ \hat{\rho}_{n,\sigma} \rightarrow \frac{2}{\pi^2} \sin(\sqrt{4\pi} \varphi(x)) + a_0^2 \frac{2}{\pi} (\partial_x \varphi(x))^2. \]

Here, \( \varphi_{\uparrow,\downarrow}(x) \) and \( P_{\uparrow,\downarrow}(x) \) are a scalar field and its conjugate momentum, respectively, related to the spin up and spin down subsystems. In deriving Eq. \[22\], the following operator product expansion relations have been used:

\[ \partial_x \varphi(x) : \sin(\sqrt{4\pi} \varphi(x) + a_0 \varphi(x)) := \frac{1}{\sqrt{\pi} a_0} \cos(\sqrt{4\pi} \varphi(x)) \cdot \]

\[ \sin(\sqrt{4\pi} \varphi(x)) : \sin(\sqrt{4\pi} \varphi(x) + a_0 \varphi(x)) := -a_0^2 \pi : (\partial_x \varphi(x))^2 - \frac{1}{2} : \cos(\sqrt{16\pi} \varphi(x)) \cdot \]

Finally, introducing the bosonic charge (\( \varphi_c \)) and spin (\( \varphi_s \)) fields

\[ \varphi_c = \frac{1}{\sqrt{2K_c}}(\varphi_\uparrow + \varphi_\downarrow), \quad P_c = \sqrt{\frac{K_c}{2}}(P_\uparrow + P_\downarrow), \]

\[ \varphi_s = \frac{1}{\sqrt{2K_s}}(\varphi_\uparrow - \varphi_\downarrow), \quad P_s = \sqrt{\frac{K_s}{2}}(P_\uparrow - P_\downarrow), \]

and converting \( \sum_0^\infty a_0 \rightarrow \int dx \) we rewrite the model Hamiltonian in terms of two decoupled quantum SG theories, \( \mathcal{H} = \mathcal{H}_c + \mathcal{H}_s \), where

\[ \mathcal{H}_c(s) = v_c(s) \int dx \left\{ \frac{1}{2} [P^2_c(s)(x) + (\partial_x \varphi_c(s))^2] + \frac{m_c(s)}{a_0^2} \cos(\sqrt{8\pi K_c(s)} \varphi_c(s)) \right\}. \]

Here we have defined

\[ K_c = (1 + g_c)^{1/2} \simeq 1 + \frac{1}{2} g_c, \quad m_c = \frac{g_c}{2}, \]

\[ K_s = (1 + g_s)^{1/2} \simeq 1 + \frac{1}{2} g_s, \quad m_s = \frac{g_s}{2}, \]

\[ v_c = \frac{v_F}{K_c} \simeq (1 - \frac{1}{2} g_c), \quad v_s = \frac{v_F}{K_s} \simeq v_F(1 - \frac{1}{2} g_s). \]

The small dimensionless coupling constants are given by:

\[ g_c = -\frac{1}{2\pi}(U + 6V + 8T^*/\pi), \]

\[ g_u = -\frac{1}{2\pi}(U - 2V + 8T^*/\pi), \]

\[ g_s = g_\perp = \frac{1}{2\pi}(U - 2V - 8T^*/\pi). \]

The relation between \( K_c, K_s \), \( m_c(m_s) \), and \( g_c(g_s) \) \( g_s \) \( g_\perp \) is universal in the weak coupling limit.

In obtaining \[27\] only nonoscillating terms of the order \( \sim a_0 \) have been kept. In addition, strongly irrelevant terms \( \sim \cos(\sqrt{5\pi K_c \varphi_c}) \cos(\sqrt{5\pi K_s \varphi_s}) \) describing umklapp scattering processes with parallel spins were omitted.

The mapping of the initial lattice Hamiltonian Eq. \[2\] into the continuum theory of quantum SG models Eq. \[25\] allows to study the ground state phase diagram of the system based on the infrared properties of the SG Hamiltonians. The corresponding behavior of the SG model is described by the pair of renormalization group equations for the effective coupling constants \( \Gamma, \Gamma \).

\[ d\Gamma_\perp/dL = -\Gamma_\perp \Gamma_\uparrow, \]

\[ d\Gamma_\uparrow/dL = -\Gamma_\perp^2, \]

\[ d\Gamma_\perp/dL = -\Gamma_\perp^2, \]

\[ d\Gamma_\uparrow/dL = -\Gamma_\perp^2, \]

where \( L = \ln(a_0) \) and \( \Gamma_i(0) = g_i \). Each pair of equations \[24\] and \[35\] describes the Kosterlitz–Thouless transition \[40\] in the charge and spin channels. The flow lines lie on the hyperbola

\[ \Gamma^2_{c(s)} - \Gamma^2_{\perp} = \mu^2_{c(s)} = g^2_{c(s)} - g^2_{\perp(s)}, \]

and – depending on the relation between the bare coupling constants \( g_{c(s)} \) and \( g_{\perp(s)} \) – exhibit two different regimes:

For \( g_c \geq |g_u| \) \( (g_s \geq |g_\perp|) \) we are in the weak coupling regime; the effective mass \( M_{c(s)} \rightarrow 0 \). The low energy (large distance) behavior of the gapless charge (spin) degrees of freedom is described by a free scalar field

\[ \mathcal{H}_{c(s)} = \frac{1}{2} v_c(s) \int dx \{(\partial_x \varphi_{c(s)})^2 + (\partial_x \varphi_{c(s)})^2\} \]

where \( \partial_x \varphi_{c(s)} = P_c(s) \).

The corresponding correlations show a power law decay

\[ \langle e^{i\sqrt{2\pi K_c \varphi'(x)} e^{-i\sqrt{2\pi K_c \varphi(x)}}} \rangle \sim |x - x'|^{-K}, \]

\[ \langle e^{i\sqrt{2\pi K \varphi'(x)} e^{-i\sqrt{2\pi K \varphi(x)}}} \rangle \sim |x - x'|^{-1/K}, \]

and the only parameter controlling the infrared behavior in the gapless regime is the fixed-point value of the effective coupling constants \( K_{c(s)} \).

For \( g_c < |g_u| \) \( (g_s < |g_\perp|) \) the system scales to the strong coupling regime; depending on the sign of the bare mass \( m_{c(s)} \) the effective mass \( M_{c(s)} \rightarrow \pm \infty \), which signals the crossover to the strong coupling regime and indicates the
dynamical generation of a commensurability gap in the charge (spin) excitation spectrum. The fields \( \varphi_c (\varphi_s) \) get ordered with the vacuum expectation values \( \langle \varphi_c \rangle \)

\[
\langle \varphi_{c(s)} \rangle = \begin{cases} \sqrt{\frac{\pi}{8K_{c(s)}}} & (m_{c(s)} > 0) \\ 0 & (m_{c(s)} < 0) \end{cases} .
\]

**IV. PHASE DIAGRAM**

Let us now consider the weak-coupling ground state phase diagram of the model Eq. (4). To clarify the symmetry properties of the various ground states of the system we use the usual order parameters describing the short wavelength fluctuations of the site-located charge-density,

\[
\Delta_{CDW} = (-1)^n \sum_\sigma \rho_{n,\sigma} \
\sim \sin(\sqrt{2\pi K_c \varphi_c}) \cos(\sqrt{2\pi K_s \varphi_s}) ,
\]

the site-located spin-density

\[
\Delta_{SDW} = \sum_\sigma \sigma \rho_{n,\sigma} 
\sim \cos(\sqrt{2\pi K_c \varphi_c}) \sin(\sqrt{2\pi K_s \varphi_s}) ,
\]

and two superconducting order parameters corresponding to singlet (\( \Delta_{SS} \)) and triplet (\( \Delta_{TS} \)) superconductivity:

\[
\Delta_{SS}(x) = R^1_\uparrow(x) L^1_\downarrow(x) - R^1_\downarrow(x) L^1_\uparrow(x) 
\sim \exp(i \sqrt{\frac{2\pi}{K_c} \theta_c}) \cos(\sqrt{2\pi K_s \varphi_s}) ,
\]

\[
\Delta_{TS}(x) = R^1_\uparrow(x) L^1_\downarrow(x) + R^1_\downarrow(x) L^1_\uparrow(x) 
\sim \exp(i \sqrt{\frac{2\pi}{K_c} \theta_c}) \sin(\sqrt{2\pi K_s \varphi_s}) .
\]

In addition we use a set of order parameters describing the short wavelength fluctuations of the bond-located charge- and spin-density

\[
\Delta_{dimer} = (-1)^n \sum_\sigma \hat{Q}_{n,n+1,\sigma} 
\sim \cos(\sqrt{2\pi K_c \varphi_c}) \cos(\sqrt{2\pi K_s \varphi_s}) ,
\]

\[
\Delta_{bd-SDW} = (-1)^n \sum_\sigma \sigma \hat{Q}_{n,n+1,\sigma} 
\sim \sin(\sqrt{2\pi K_c \varphi_c}) \sin(\sqrt{2\pi K_s \varphi_s}) .
\]

A. The \( SU(2) \otimes SU(2) \) symmetric case

We first consider the \( SU(2) \otimes SU(2) \) symmetric case for \( 2k^* + T^* = 0 \). In this case the coupling constants parametrizing the charge and spin degrees of freedom are given by

\[
g_c = g_u = \frac{1}{\pi V_F} (U + 8T^*/\pi) ,
\]

\[
g_s = g_\perp = \frac{1}{\pi V_F} (U - 8T^*/\pi) .
\]

Although the given parameters are determined within the weak-coupling approach (|\( g_i \) | \( \ll 1 \)) the relations Eqs. (43) are universal and determined by the symmetries of the model only. This strongly restricts the scaling trajectories along the separatrix \( \mu = 0 \) (see Fig. 1). The \( SU(2) \otimes SU(2) \) is easily seen from Eqs. (43); each channel is characterized by one parameter \( g_c \) and \( g_s \), respectively, and the electron-hole transformation Eq. (8) only interchanges the bare values of these parameters.

![Figure 1](image_url)

**FIG. 1.** The renormalization-group flow diagram; the arrows denote the direction of flow with increasing length scale.

It follows from (47) that for \( U > -8T^*/\pi \) there is a gap in the charge excitation spectrum, and the \( \varphi_c \) field is ordered with vacuum expectation value \( \langle \varphi_c \rangle = 0 \). In the weak-coupling regime for \( U \leq -8T^*/\pi \) where \( M_s \to 0 \), gapless charge excitations are described by the free bose field with the fixed-point value \( K^*_c = 1 \).

The spin sector is massive for \( U < 8T^*/\pi \). The dynamical generation of a gap in the spin sector is accompanied by the ordering of the \( \varphi_s \) field with vacuum expectation value \( \langle \varphi_s \rangle = 0 \). For \( U > 8T^*/\pi \) the spin sector is gapless, \( M_s \to 0 \) and the fixed-point value \( K^*_s = 1 \).
We next consider the case $T^* < 0$ (see Fig. 2b). The spin gap regime is realized for $U < -8 |T^*|/\pi < 0$ and the charge gap regime for $U > 8 |T^*|/\pi > 0$. Therefore, the properties of the model in the sectors $A_1$ ($U > 8 |T^*|/\pi$) and $C_1$ ($U < -8 |T^*|/\pi$) are the same as in the corresponding $A$ and $C$ sectors in the case of $T^* > 0$.

However, for $-8 |T^*|/\pi < U < 8 |T^*|/\pi$ both, the charge and the spin channel are gapless. The fixed point values of the LL parameters are given by

$$K_c^* = K_s^* = 1.$$ 

Using Eqs. (41)-(46) and (38)-(39) one obtains that all correlations show an identical $\sim |x - x'|^{-2}$ decay at large distances in this case.

**B. Effects of $V$**

Let us now consider the weak coupling phase diagram of the model Eq. (3) for $V \neq 0$. From Eqs. (31)-(33) one obtains that there is a gap in the spin excitation spectrum for $U < 2V + 8T^*/\pi$. The charge excitation spectrum is gapped for $U > 2|V| - 8T^*/\pi$ and - in the case of repulsive nn interaction ($V > 0$) - for $U < 2V - 8T^*/\pi$. The line $U = 2|V| - 8T^*/\pi$ corresponds to a metallic LL phase. This determines five different sectors in the phase diagram.

We start with the $T^* > 0$ case (see Fig. 3a).

**Sector A**: $U > 2V + 8T^*/\pi$. This is the sector dominated by on-site repulsion. The properties of the system in this sector coincide with that of sector $A$ for the $V = 0$ case. The line $U = 2V + 8T^*/\pi$ marks the transition into the spin gap regime.

**Sector B**: $|U - 2V| < 8T^*/\pi$, $V > -4T^*/\pi$. In this sector both channels are massive and the LRO dimerized phase is realized. The line $U = 2V - 8T^*/\pi$ corresponds to a nonmagnetic metallic phase. Along this line the charge gap is zero, while the spin gap remains finite, and $K_c \simeq 1 - 2V/\pi t < 1$. The TS instability is suppressed, while the SS correlations decay at large distances faster than the density-density correlations

$$\langle \Delta_{SS}(x)\Delta_{SS}(x') \rangle \sim |x - x'|^{-1/K_c}.$$ 

**Sector $C_1$**: $U < 2V - 8T^*/\pi$ and $V > 0$. A gap in the charge excitation spectrum opens once again; however, in this sector the vacuum expectation value of the charge field is $\langle \phi_c \rangle = \sqrt{\pi/8K_c}$. The spin sector is gapped with $\langle \phi_s \rangle = 0$. Using Eqs. (41)-(46) one obtains a LRO CDW in the ground state:

$$\langle \Delta_{CDW}(x)\Delta_{CDW}(x') \rangle \sim \text{constant.}$$
Finally, we analyze the case $T^* < 0$ (see Fig. 3b). The phase diagram once again consists of five different sectors:

Sectors A, C1, C2, and D are identical to the corresponding sectors for the $T^* > 0$ case. Particular is sector B: $|U - 2V| < 8T^*/\pi$ and $V > 0$. In this sector the spin spectrum is gapless while the charge excitation spectrum is massive and the vacuum expectation value of the ordered charge field is $\langle \varphi_c \rangle = \sqrt{\pi}/8K_c$. Using Eqs. (11)-(14) one obtains in this sector an insulating phase with dominating CDW and $bd - SDW$ instabilities showing a power-law decay at large distances

$$\langle \Delta_{CDW}(x)\Delta_{CDW}(x') \rangle = \langle \Delta_{bd-SDW}(x)\Delta_{bd-SDW}(x') \rangle \sim |x - x'|^{-1}$$

with the critical indices governed by the $SU(2)$–spin symmetry of the model.

V. DISCUSSION AND SUMMARY

In this paper we have studied the one-dimensional extended Hubbard model with CH interactions at half-filling. We have demonstrated that the CH interaction can lead to bond located ordering in the ground state. Along the line $U = 2V > 0$, for a "repulsive" three-body coupling $(T^* > 0)$, the LRO dimerized phase corresponding to an enhanced Peierls instability in the system, is realized. In the case of an "attractive" three-body term $(T^* < 0)$ the $bd - SDW$ phase corresponding to a bond located staggered magnetization is – together with the CDW – the most divergent instability in the system. For $T^* \to 0$ the sector with new phases shrinks to the line $U = 2V$ and the ground state phase diagram of the extended Hubbard model is recovered.

Although the phase diagram was studied within the continuum-limit approach, assuming the bare-values of the coupling constants much less than the bandwidth, the phase diagram is strongly controlled by the symmetry of the model. This allows to suppose that the features of the phase diagram will persist also in the limit $U, V \gg t$, as far as the ground state phase diagram of the extended Hubbard model is essentially the same in both limits.

However, the weak CH regime is not continuously connected to the ground states at $|t^*| = t$ implying the existence of father $t^*$ ($T^*$) driven phase transitions. These additional transitions arise only if the important finite bandwidth effects are included which is beyond the scope of our approach.

For $V = 0$ and $U = U_c = 8T^*/\pi$ the SDW insulator-metal transition is in qualitative agreement with results of numerical studies. However, contrary to the numerical results showing a TS phase for $U < U_c$, our results indicate a metallic LL phase in this case, with identically
divergent density-density and superconducting instabilities due to the SU(2) ⊗ SU(2) symmetry of the model. Moreover, due to the SU(2)-spin symmetry of the model, the dynamical generation of a spin gap for $U < -U_c < 0$, supports only the SS instabilities.

For $V \neq 0$ we find that the metallic phase shrinks due to the repulsive nn coupling up to the line $U = 2V + 8/T^\ast |/\pi$. There is no superconductivity for $V > 0$ in the weak coupling phase diagram.

ACKNOWLEDGMENTS

G. J. gratefully acknowledges the kind hospitality at the Center for Electronic Correlations and Magnetism at the University of Augsburg. This work was financially supported by the Deutsche Forschungsgemeinschaft.

1 Permanent Address: Institute of Physics, Georgian Academy, Tamarashvili 6, Tbilisi 380077, Georgia. Electronic address: japa@iphi.hep2.edu.ge

[1] M.E. Foglio and L.M. Falicov, Phys. Rev. B 20, 4554 (1979).
[2] J. Hubbard, Proc. Roy. Soc. London A 276, 238 (1963).
[3] M.E. Simon and A. Aligia, Phys. Rev. B 48, 7471 (1993).
[4] G. Santoro, M. Airoldy, N. Manini, A. Parola, and E. Tosatti, Phys. Rev. Lett. 74, 4039 (1995).
[5] S. Kivelson, W.-P. Su, J.R. Schrieffer, and A.J. Heeger, Phys. Rev. B 51, 13744 (1995).
[6] L. Arrachea, A. Aligia, E. Gagliano, K. Hallberg, and C. Balseiro, Phys. Rev. B 50, 16044 (1994).
[7] A. Aligia, L. Arrachea, and E. Gagliano, Phys. Rev. B 51, 13744 (1995).
[8] E. Gagliano, A. Aligia, L. Arrachea, and M. Avignon, Phys. Rev. B 51, 14012 (1995).
[9] L. Arrachea, E. Gagliano, and A. Aligia, Phys. Rev. B 55, 1173 (1997).
[10] K. Michielsen and H. de Raedt, Int. J. Mod. Phys. B 11, 1311 (1997).
[11] M.E. Simon, A. Aligia, and E. Gagliano, Phys. Rev. B 56, 5637 (1997).
[12] A. Aligia, E. Gagliano, L. Arrachea and K. Hallberg, preprint cond-mat/9805198.
[13] L. Arrachea and A. Aligia, preprint cond-mat/9803034.
[14] M. Airoldy and A. Parola, Phys. Rev. B 51, 16327 (1995).
[15] G.I. Japaridze, Phys. Lett. A 201, 239 (1995).
[16] G.I. Japaridze and E. Müller-Hartmann, J. Phys. Cond. Mat. 9, 10509 (1997).
[17] V.J. Emery, in Highly Conducting One-Dimensional Solids, edited by J.T. Devreese, R.P. Evrard, and V.E. Van Doren, Plenum, New York (1979); J. Solyom, Adv. Phys. 28, 201 (1979).
[18] J. Voit, Phys. Rev. B 45, 4027 (1992).
[19] J.E. Hirsch, Phys. Rev. Lett. 53, 2327 (1984); Phys. Rev. B 31, 6022 (1985); J. Cannon and E. Fradkin, ibid. 41, 9435 (1989); J. Cannon, R. Scaletter, and E. Fradkin, ibid. 44, 5995 (1991); G.P. Zhang, ibid. 56, 9189 (1997).
[20] H. Frahm and V.E. Korepin, Phys. Rev. B 52, 10533 (1990); N. Kawakami and S.-K. Yang, Phys. Lett. A 148, 359 (1990).
[21] L. Arrachea, A. Aligia, and E. Gagliano, Phys. Rev. Lett. 76, 4396 (1996).
[22] R. Bariev, A. Klümper, A. Schadschneider, and J. Zittartz, J. Phys. A 26, 4863 (1993); ibid. 26, 1249 (1993).
[23] I. N. Kamiuchikov, Phys. Rev. Lett. 73, 1130 (1994).
[24] L. Quaisser, A. Schadschneider, and J. Zittartz, Europhys. Lett. 32, 85 (1995).
[25] R. Bariev, A. Klümper, A. Schadschneider, and J. Zittartz, Europhys. Lett. 32, 179 (1995).
[26] A. Schadschneider, G. Su, and J. Zittartz, Z. Phys. B 102, 397 (1997).
[27] L. Arrachea, A. Aligia, E. Gagliano, K. Hallberg, and C. Balseiro, Phys. Rev. B 50, 16044 (1994).
[28] A. Aligia, L. Arrachea, and E. Gagliano, Phys. Rev. B 51, 13744 (1995).
[29] E. Gagliano, A. Aligia, L. Arrachea, and M. Avignon, Phys. Rev. B 51, 14012 (1995).
[30] L. Arrachea, E. Gagliano, and A. Aligia, Phys. Rev. B 55, 1173 (1997).
[31] K. Michielsen and H. de Raedt, Int. J. Mod. Phys. B 11, 1311 (1997).
[32] M.E. Simon, A. Aligia, and E. Gagliano, Phys. Rev. B 56, 5637 (1997).
[33] A. Aligia, E. Gagliano, L. Arrachea and K. Hallberg, preprint cond-mat/9805198.
[34] L. Arrachea and A. Aligia, preprint cond-mat/9803034.
[35] M. Airoldy and A. Parola, Phys. Rev. B 51, 16327 (1995).
[36] G.I. Japaridze, Phys. Lett. A 201, 239 (1995).
[37] G.I. Japaridze and E. Müller-Hartmann, J. Phys. Cond. Mat. 9, 10509 (1997).
[38] V.J. Emery, in Highly Conducting One-Dimensional Solids, edited by J.T. Devreese, R.P. Evrard, and V.E. Van Doren, Plenum, New York (1979); J. Solyom, Adv. Phys. 28, 201 (1979).
[39] J. Voit, Phys. Rev. B 45, 4027 (1992).
[40] J.E. Hirsch, Phys. Rev. Lett. 53, 2327 (1984); Phys. Rev. B 31, 6022 (1985); J. Cannon and E. Fradkin, ibid. 41, 9435 (1989); J. Cannon, R. Scaletter, and E. Fradkin, ibid. 44, 5995 (1991); G.P. Zhang, ibid. 56, 9189 (1997).
[41] H. Frahm and V.E. Korepin, Phys. Rev. B 52, 10533 (1990); N. Kawakami and S.-K. Yang, Phys. Lett. A 148, 359 (1990).
[42] For a recent review see A.O. Gogolin, A.A. Nersesyan and A.M. Tsvelik, Bosonization and strongly correlated systems, Cambridge University Press (1998).
[43] A. Luther and V.J. Emery, Phys. Rev. Lett. 33, 589 (1974).
[44] P. Wiegmann, J. Phys. C 11, 1583 (1978); D. Boyanovsky, J. Phys. A 22, 2601 (1989).
[45] J.M. Kosterlitz and D. Thouless, J. Phys. C: Solid State Phys. 6, 1181 (1973); ibid. 7, 1046 (1974).
[46] K.A. Muttalib and V.J. Emery, Phys. Rev. Lett. 57, 1370 (1986); T. Giamarchi and H.J. Schulz, Jour. Phys. (Paris) 49, 819 (1988); Phys. Rev. B 33, 2066 (1988).
[47] A.A. Nersesyan, Phys. Lett. A 153, 49 (1991).