

Weak-coupling phase diagram of the extended Hubbard model with correlated-hopping interaction

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A one-dimensional model of interacting electrons with on-site U , nearest-neighbor V , and correlated-hopping 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 $T^* < 0$, $|U - 2V| < 8|T^*|/\pi$. The general ground-state phase diagram including insulating, metallic, and superconducting phases is discussed. [S0163-1829(99)07119-2]

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) interaction¹⁻³⁷ are the subject of current studies. In addition to the usual interaction between electrons on the same site (U) and/or on nearest-neighbor (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 Hamiltonian² 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^{1,3,4} 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.¹ 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.⁵⁻¹⁰

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.¹¹ 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 η -pairing type.¹² 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,¹⁵ the exact solution for particular values of coupling constants, and by numerical techniques.¹⁶⁻²¹ Several exactly solvable one-dimensional (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

$$\begin{aligned} \mathcal{H} = & t_{eh} \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} (1 - \hat{\rho}_{n,-\sigma}) (1 - \hat{\rho}_{n+1,-\sigma}) \\ & + t_{ed} \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} \hat{\rho}_{n,-\sigma} \hat{\rho}_{n+1,-\sigma} + t_{dd} \\ & \times \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} (\hat{\rho}_{n,-\sigma} + \hat{\rho}_{n+1,-\sigma} - 2\hat{\rho}_{n,-\sigma} \hat{\rho}_{n+1,-\sigma}) \\ & + \frac{1}{2} U \sum_{n,\sigma} \hat{\rho}_{n,\sigma} \hat{\rho}_{n,-\sigma} + V \sum_n \hat{\rho}_n \hat{\rho}_{n+1}, \end{aligned} \quad (1)$$

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

$$\begin{aligned} \mathcal{H} = & -t \sum_{n,\sigma} (c_{n,\sigma}^\dagger c_{n+1,\sigma} + c_{n+1,\sigma}^\dagger c_{n,\sigma}) - \mu \sum_{n,\sigma} c_{n,\sigma}^\dagger c_{n,\sigma} \\ & + \frac{1}{2} U \sum_{n,\sigma} \hat{\rho}_{n,\sigma} \hat{\rho}_{n,-\sigma} + V \sum_n \hat{\rho}_n \hat{\rho}_{n+1} \\ & + t^* \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} (\hat{\rho}_{n,-\sigma} + \hat{\rho}_{n+1,-\sigma}) \\ & + T^* \sum_{n,\sigma} \hat{Q}_{n,n+1,\sigma} \hat{\rho}_{n,-\sigma} \hat{\rho}_{n+1,-\sigma}. \end{aligned} \quad (2)$$

Here $t = -t_{ed}$, $t^* = t_{eh} - t_{dd}$, and $T^* = 2t_{dd} - t_{eh} - t_{ed}$. There are N_e particles, N_0 sites, and the band filling ν

$=N_e/2N_0$ is controlled by the chemical potential μ .

The 2D version of the Hamiltonian (1) has been derived by Simon and Aligia 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.²⁸⁻³⁷ 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 are in qualitative agreement with results for the standard CH model ($T^* = 0$).¹³⁻¹⁵ There is a transition into a superconducting phase for particular band fillings and sufficiently small on-site repulsion.^{28,37} The effective interaction originating from the t^* term that appears in the continuum-limit theory, is given by $t^* \cos(\pi\nu)$.¹⁵ 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.^{29,30,21,32} The nature of superconducting instabilities in the metallic phase was investigated numerically and within a mean-field approach.³³⁻³⁶ Recently, also the possibility for realizing triplet superconductivity (TS) in the ground state of the model (2) at half filling was studied.^{35,36}

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*.^{38,39} 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,⁴⁰ for $|U - 2V| < 8T^*/\pi$ and $V > -4T^*/\pi$ the long-range-ordered (LRO) dimerized ground state with order parameter

$$\Delta_{dimer} = (-1)^n \sum_{\sigma} \hat{Q}_{n,n+1,\sigma} \quad (3)$$

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

$$\Delta_{bd-SDW} = (-1)^n \sum_{\sigma} \sigma \hat{Q}_{n,n+1,\sigma} \quad (4)$$

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

The paper is organized as follows: In Sec. II the symmetry of the model is reviewed. In Sec. III the continuum-limit bosonized version of the model is constructed. In Sec. IV, we discuss the weak-coupling phase diagram. Finally, Sec. 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 $\frac{1}{2}$ -filled extended Hubbard model is well studied:⁴⁰⁻⁴³ 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 $U = 2V$ line corresponds to a transition from the SDW phase (for $U > 2V$) into an insulating LRO CDW phase for $U < 2V$.⁴⁰⁻⁴³ 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.⁴¹

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.^{11,15}

Let us first consider the symmetry aspect. The three generators of the spin-SU(2) algebra

$$S^+ = \sum_n c_{n,\uparrow}^\dagger c_{n,\downarrow}, \quad S^- = \sum_n c_{n,\downarrow}^\dagger c_{n,\uparrow},$$

$$S^z = \sum_n \frac{1}{2} (c_{n,\uparrow}^\dagger c_{n,\uparrow} - c_{n,\downarrow}^\dagger c_{n,\downarrow}), \quad (5)$$

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

The electron-hole transformation

$$c_{n,\sigma} \rightarrow (-1)^n c_{n,\sigma}^\dagger, \quad (6)$$

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

$$\tilde{t} = t - 2t^* - T^*, \quad \tilde{t}^* = -t^* - T^* \quad (7)$$

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

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

$$c_{n,\uparrow} \rightarrow c_{n,\uparrow}^\dagger$$

$$c_{n,\downarrow} \rightarrow (-1)^n c_{n,\downarrow}^\dagger, \quad (8)$$

interchanges the charge and spin degrees of freedom and converts

$$\mathcal{H}(t, U, T^*) \rightarrow \mathcal{H}(t, -U, T^*). \quad (9)$$

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) symmetry¹⁸ with generators

$$\eta^+ = \sum_n (-1)^n c_{n,\uparrow}^\dagger c_{n,\downarrow}^\dagger, \quad \eta^- = \sum_n (-1)^n c_{n,\downarrow} c_{n,\uparrow},$$

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

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.⁴⁴

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,⁴⁵ for clarity we briefly sketch the most important points and focus our attention on the three-body term.

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 $\pm k_F$ ($k_F = \pi/2a_0$, where a_0 is the lattice spacing) we linearize the spectrum around these points and obtain two species (for each spin projection σ) of fermions $R_\sigma(n)$ and $L_\sigma(n)$ which describe excitations with dispersion relations $E = \pm v_F p$. Here, $v_F = 2ta_0$ 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:

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

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

$$\begin{aligned} R_\sigma(n) &\rightarrow \sqrt{a_0} R_\sigma(x = na_0), \\ L_\sigma(n) &\rightarrow \sqrt{a_0} L_\sigma(x = na_0). \end{aligned} \quad (12)$$

In terms of the continuum fields the free Hamiltonian reads

$$\mathcal{H}_0 = E_0 - i v_F \sum_\sigma \int dx [:R_\sigma^\dagger \partial_x R_\sigma : - :L_\sigma^\dagger \partial_x L_\sigma :], \quad (13)$$

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 independent (in the weak-coupling limit) 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

$$\begin{aligned} \hat{\rho}_{n,\sigma} - \frac{1}{2} &\equiv : \hat{\rho}_{n,\sigma} : \\ &= a_0 \{ [:R_\sigma^\dagger(x) R_\sigma(x) : + :L_\sigma^\dagger(x) L_\sigma(x) :] \\ &\quad + (-1)^n [R_\sigma^\dagger(x) L_\sigma(x) + L_\sigma^\dagger(x) R_\sigma(x)] \}, \end{aligned} \quad (14)$$

$$\begin{aligned} : \hat{Q}_{n,n+1;\sigma} : &\equiv \hat{Q}_{n,n+1;\sigma} - \frac{2}{\pi} \\ &= 2a_0 i (-1)^{n+1} [R_\sigma^\dagger(x) L_\sigma(x) - L_\sigma^\dagger(x) R_\sigma(x)] \\ &\quad + O(a_0^2). \end{aligned} \quad (15)$$

The second step is to use the standard bosonization expressions for fermionic bilinears⁴⁶

$$-i [:R_\sigma^\dagger \partial_x R_\sigma : - :L_\sigma^\dagger \partial_x L_\sigma :] \rightarrow \frac{1}{2} \{ P_\sigma^2(x) + (\partial_x \phi_\sigma)^2 \}, \quad (16)$$

$$:R_\sigma^\dagger(x) R_\sigma(x) : + :L_\sigma^\dagger(x) L_\sigma(x) : \rightarrow \frac{1}{\sqrt{\pi}} \partial_x \phi_\sigma(x), \quad (17)$$

$$:R_\sigma^\dagger(x) R_\sigma(x) : - :L_\sigma^\dagger(x) L_\sigma(x) : \rightarrow -\frac{1}{\sqrt{\pi}} P_\sigma(x), \quad (18)$$

$$R_\sigma^\dagger(x) L_\sigma(x) \rightarrow -\frac{i}{2\pi a_0} \exp[-i\sqrt{4\pi}\phi_\sigma(x)]. \quad (19)$$

We thereby obtain

$$: \hat{\rho}_{n,\sigma} : \rightarrow a_0 \left\{ \frac{1}{\sqrt{\pi}} \partial_x \phi_\sigma - (-1)^n \frac{1}{\pi a_0} \sin(\sqrt{4\pi}\phi_\sigma) \right\}, \quad (20)$$

$$: \hat{Q}_{n,n+1;\sigma} : \rightarrow (-1)^{n+1} \frac{2}{\pi} \cos(\sqrt{4\pi}\phi_\sigma) + \dots, \quad (21)$$

$$\begin{aligned} \hat{\rho}_{n,\sigma}::\hat{\rho}_{n+1,\sigma}:: &\rightarrow +a_0^2 \left\{ \frac{2}{\pi} (\partial_x \varphi_\sigma)^2 + \frac{1}{2\pi^2 a_0^2} \cos(\sqrt{16\pi} \varphi_\sigma) \right. \\ &\left. + (-1)^n \frac{2}{\pi^2 a_0^2} \cos(\sqrt{4\pi} \varphi_\sigma) \right\} + \dots \end{aligned} \quad (22)$$

Here, $\varphi_{\sigma=\uparrow,\downarrow}(x)$ and $P_{\sigma=\uparrow,\downarrow}(x)$ 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:

$$\begin{aligned} \partial_x \varphi(x)::\sin[\sqrt{4\pi} \varphi(x+a_0)]: & \\ = \frac{1}{\sqrt{\pi a_0}}::\cos[\sqrt{4\pi} \varphi(x)]: + \dots, & \quad (23) \end{aligned}$$

$$\begin{aligned} \sin[\sqrt{4\pi} \varphi(x)]:\sin[\sqrt{4\pi} \varphi(x+a_0)]: & \\ = \text{const} - \frac{1}{2}::\cos[\sqrt{16\pi} \varphi(x)]: - a_0^2 \pi::[\partial_x \varphi(x)]^2:: + \dots \end{aligned} \quad (24)$$

In Eqs. (21)–(24) dots denote the higher order terms in expansion with respect to a_0 .

Finally, introducing the bosonic charge (φ_c) and spin (φ_s) fields

$$\varphi_c = \frac{1}{\sqrt{2K_c}}(\varphi_\uparrow + \varphi_\downarrow), \quad P_c = \sqrt{\frac{K_c}{2}}(P_\uparrow + P_\downarrow), \quad (25)$$

$$\varphi_s = \frac{1}{\sqrt{2K_s}}(\varphi_\uparrow - \varphi_\downarrow), \quad P_s = \sqrt{\frac{K_s}{2}}(P_\uparrow - P_\downarrow), \quad (26)$$

converting $\sum_n a_0 \rightarrow \int dx$ and taking the limit $a_0 \rightarrow 0$, $t \rightarrow \infty$, $2ta_0 = v_F$ we rewrite the model Hamiltonian in the following way:

$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_s + \mathcal{H}_{cs},$$

where

$$\mathcal{H}_c = v_c \int dx \left\{ \frac{1}{2} [P_c^2(x) + (\partial_x \varphi_c)^2] + \frac{m_c}{a_0^2} \cos(\sqrt{8\pi K_c} \varphi_c) \right\}, \quad (27)$$

$$\mathcal{H}_s = v_s \int dx \left\{ \frac{1}{2} [P_s^2(x) + (\partial_x \varphi_s)^2] + \frac{m_s}{a_0^2} \cos(\sqrt{8\pi K_s} \varphi_s) \right\}, \quad (28)$$

$$\mathcal{H}_{cs} = v_F \frac{M_{cs}}{a_0^2} \int dx \cos(\sqrt{8\pi K_c} \varphi_c) \cos(\sqrt{8\pi K_s} \varphi_s). \quad (29)$$

Here, we have defined

$$K_c = (1 - g_c)^{-1/2} \approx 1 + \frac{1}{2} g_c, \quad m_c = \frac{g_u}{2\pi}, \quad (30)$$

$$K_s = (1 - g_s)^{-1/2} \approx 1 + \frac{1}{2} g_s, \quad m_s = \frac{g_\perp}{2\pi}, \quad (31)$$

$$v_c = \frac{v_F}{K_c} \approx \left(1 - \frac{1}{2} g_c\right), \quad v_s = \frac{v_F}{K_s} \approx v_F \left(1 - \frac{1}{2} g_s\right), \quad (32)$$

$$M_{cs} = \frac{g_{cs}}{\pi}. \quad (33)$$

The small dimensionless coupling constants are given by

$$g_c = -\frac{1}{2\pi t} (U + 6V + 8T^*/\pi), \quad (34)$$

$$g_u = -\frac{1}{2\pi t} (U - 2V + 8T^*/\pi), \quad (35)$$

$$g_s = g_\perp = \frac{1}{2\pi t} (U - 2V - 8T^*/\pi), \quad (36)$$

$$g_{cs} = \frac{1}{2\pi t} (V + 2T^*/\pi). \quad (37)$$

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

As it follows from Eqs. (27)–(37) the three-body interaction contributes to marginally relevant scattering processes with scaling dimensionalities $d_c = 2K_c \approx 2$ and $d_s = 2K_s \approx 2$ given by \mathcal{H}_c and \mathcal{H}_s as well as to the spin-charge coupling given by the \mathcal{H}_{cs} term. The scaling dimensionality of the latter is $d = d_c + d_s \approx 4$, and therefore, the spin-charge coupling is strongly irrelevant in the weak-coupling limit. From numerical studies of the extended $U-V$ Hubbard model^{42,43} it is known that this interaction does not lead to qualitative change in the phase diagram at least for $V \leq 2.5t$, far apart the range of applicability of our approach. In what follows, the \mathcal{H}_{cs} term will be omitted. In this case, performed mapping of the initial lattice Hamiltonian Eq. (2) into the continuum theory of two decoupled quantum SG models Eqs. (27)–(28) 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 Γ_i (Ref. 47)

$$\begin{aligned} d\Gamma_u/dL &= -\Gamma_c \Gamma_u, \\ d\Gamma_c/dL &= -\Gamma_u^2, \end{aligned} \quad (38)$$

$$\begin{aligned} d\Gamma_\perp/dL &= -\Gamma_s \Gamma_\perp, \\ d\Gamma_s/dL &= -\Gamma_\perp^2, \end{aligned} \quad (39)$$

where $L = \ln(a_0)$ and $\Gamma_i(0) = g_i$. Each pair of Eqs. (38) and (39) describes the Kosterlitz–Thouless transition⁴⁸ in the charge and spin channels. The flow lines lie on the hyperbolas

$$\Gamma_{c(s)}^2 - \Gamma_{u(\perp)}^2 = \mu_{c(s)}^2 = g_{c(s)}^2 - g_{u(\perp)}^2, \quad (40)$$

and—depending on the relation between the bare coupling constants $g_{c(s)}$ and $g_{u(\perp)}$ —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

$$\mathcal{H}_{c(s)} = \frac{1}{2} v_{c(s)} \int dx \{ (\partial_x \theta_{c(s)})^2 + (\partial_x \varphi_{c(s)})^2 \}, \quad (41)$$

where $\partial_x \theta_{c(s)} = P_{c(s)}$.

The corresponding correlations show a power law decay

$$\langle e^{i\sqrt{2\pi K} \varphi(x)} e^{-i\sqrt{2\pi K} \varphi(x')} \rangle \sim |x-x'|^{-K}, \quad (42)$$

$$\langle e^{i\sqrt{2\pi/K} \theta(x)} e^{-i\sqrt{2\pi/K} \theta(x')} \rangle \sim |x-x'|^{-1/K}, \quad (43)$$

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 φ_c (φ_s) get ordered with the vacuum expectation values⁴⁹

$$\langle \varphi_{c(s)} \rangle = \begin{cases} \sqrt{\frac{\pi}{8K_{c(s)}}} & (m_{c(s)} > 0) \\ 0 & (m_{c(s)} < 0). \end{cases} \quad (44)$$

IV. PHASE DIAGRAM

Let us now consider the weak-coupling ground-state phase diagram of the model Eq. (2). 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,

$$\Delta_{CDW} = (-1)^n \sum_{\sigma} \rho_{n,\sigma} \sim \sin(\sqrt{2\pi K_c} \varphi_c) \cos(\sqrt{2\pi K_s} \varphi_s), \quad (45)$$

the *site*-located spin-density

$$\Delta_{SDW} = \sum_{\sigma} \sigma \rho_{n,\sigma} \sim \cos(\sqrt{2\pi K_c} \varphi_c) \sin(\sqrt{2\pi K_s} \varphi_s), \quad (46)$$

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

$$\begin{aligned} \Delta_{SS}(x) &= R_{\uparrow}^{\dagger}(x) L_{\downarrow}^{\dagger}(x) - R_{\downarrow}^{\dagger}(x) L_{\uparrow}^{\dagger}(x) \\ &\sim \exp\left(i \sqrt{\frac{2\pi}{K_c}} \theta_c\right) \cos(\sqrt{2\pi K_s} \varphi_s), \end{aligned} \quad (47)$$

$$\begin{aligned} \Delta_{TS}(x) &= R_{\uparrow}^{\dagger}(x) L_{\downarrow}^{\dagger}(x) + R_{\downarrow}^{\dagger}(x) L_{\uparrow}^{\dagger}(x) \\ &\sim \exp\left(i \sqrt{\frac{2\pi}{K_c}} \theta_c\right) \sin(\sqrt{2\pi K_s} \varphi_s). \end{aligned} \quad (48)$$

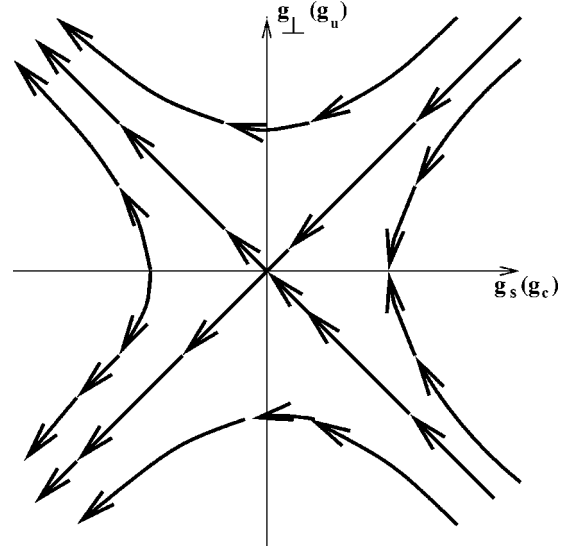


FIG. 1. The renormalization-group flow diagram; the arrows denote the direction of flow with increasing length scale.

In addition we use a set of order parameters⁵⁰ describing the short wavelength fluctuations of the *bond*-located charge and spin density

$$\begin{aligned} \Delta_{dimer} &= (-1)^n \sum_{\sigma} \hat{Q}_{n,n+1,\sigma} \\ &\sim \cos(\sqrt{2\pi K_c} \varphi_c) \cos(\sqrt{2\pi K_s} \varphi_s), \end{aligned} \quad (49)$$

$$\begin{aligned} \Delta_{bd-SDW} &= (-1)^n \sum_{\sigma} \sigma \hat{Q}_{n,n+1,\sigma} \\ &\sim \sin(\sqrt{2\pi K_c} \varphi_c) \sin(\sqrt{2\pi K_s} \varphi_s). \end{aligned} \quad (50)$$

With the results of the previous section for the excitation spectrum and the behavior of the corresponding fields Eqs. (42)–(44) we now analyze the ground-state phase diagram.

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

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

$$\begin{aligned} g_c = g_u &= -\frac{1}{\pi v_F} (U + 8T^*/\pi), \\ g_s = g_\perp &= \frac{1}{\pi v_F} (U - 8T^*/\pi). \end{aligned} \quad (51)$$

Although the given parameters are determined within the weak-coupling approach ($|g_i| \ll 1$) the relations Eqs. (51) 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. (51): 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.

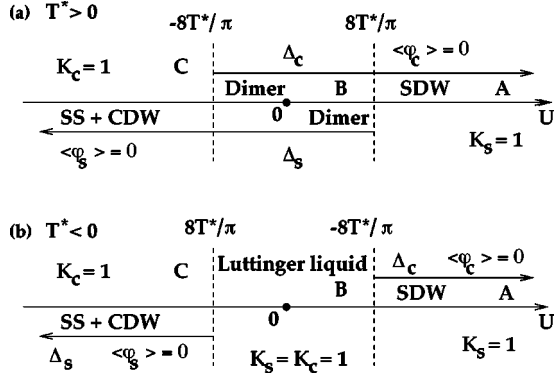


FIG. 2. Phase diagram of the model Hamiltonian Eq. (2) for the case of a half-filled band: (a) $V=0$, $T^*>0$ and (b) $T^*<0$.

It follows from Eq. (51) that for $U > -8T^*/\pi$ there is a gap in the charge excitation spectrum, and the φ_c field is ordered with vacuum expectation value $\langle \varphi_c \rangle = 0$. In the weak-coupling regime for $U \leq -8T^*/\pi$ where $M_c \rightarrow 0$, 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 φ_s field with vacuum expectation value $\langle \varphi_s \rangle = 0$. For $U > 8T^*/\pi$, the spin sector is gapless, $M_s \rightarrow 0$ and the fixed-point value $K_s^* = 1$.

There are three different sectors in the phase diagram. We start with a discussion of the $T^*>0$ case [see Fig. 2(a)].

Sector A: $U \geq 8T^*/\pi$. There is a gap in the charge excitation spectrum. The charge field is ordered $\langle \varphi_c \rangle = 0$. The spin excitation spectrum is gapless. The fixed-point value of the parameter $K_s^* = 1$. Using Eqs. (45)–(50) and (42) and (43) one obtains that the superconducting and CDW instabilities are suppressed. The SDW and *Dimer* correlations show an identical power-law decay at large distances

$$\langle \Delta_{SDW}(x)\Delta_{SDW}(x') \rangle = \langle \Delta_{dimer}(x)\Delta_{dimer}(x') \rangle \sim |x-x'|^{-1}. \quad (52)$$

The coexistence of the SDW and *Dimerization* instabilities in the repulsive Hubbard model is the mechanism for the Spin-Peierls transition at $U \gg t$.

Sector B: $8T^*/\pi > U > -8T^*/\pi$. For $U < 8T^*/\pi$ a spin gap opens. The charge and spin channels are gapped and both, charge and spin fields are ordered, $\langle \varphi_c \rangle = \langle \varphi_s \rangle = 0$. In this case, the LRO dimerized phase

$$\langle \Delta_{dimer}(x)\Delta_{dimer}(x') \rangle \sim \text{const} \quad (53)$$

is realized in the ground state.

Sector C: $U \leq -8T^*/\pi$. At $U = -8T^*/\pi$ the charge gap closes. For $U \leq -8T^*/\pi$ the phase diagram is similar to that of the half-filled attractive Hubbard model, i.e., there is a gap in the spin excitation spectrum. Due to the SU(2)-spin symmetry the vacuum expectation value $\langle \varphi_s \rangle = 0$. The SDW and TS fluctuations are completely suppressed. The charge excitation spectrum is gapless and the fixed-point value of the parameter K_c [due to the SU(2)-charge symmetry] is $K_c^* = 1$. The CDW, SS, and *Dimer* correlations show an identical power-law decay at large distances

$$\begin{aligned} \langle \Delta_{CDW}(x)\Delta_{CDW}(x') \rangle &= \langle \Delta_{SS}(x)\Delta_{SS}(x') \rangle \\ &= \langle \Delta_{dimer}(x)\Delta_{dimer}(x') \rangle \sim |x-x'|^{-1}. \end{aligned} \quad (54)$$

We next consider the case $T^*<0$ [see Fig. 2(b)]. 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. (45)–(50) and (42) and (43) 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. (2) for $V \neq 0$. From Eqs. (34)–(36) 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. 3(a)].

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 non-magnetic metallic phase. Along this line the charge gap is zero, while the spin gap remains finite, and $K_c \approx 1 - 2V/\pi t < 1$. The TS instability is suppressed, while the SS correlations

$$\langle \Delta_{SS}(x)\Delta_{SS}(x') \rangle \sim |x-x'|^{-1/K_c} \quad (55)$$

decay at large distances faster than the density-density correlations

$$\begin{aligned} \langle \Delta_{CDW}(x)\Delta_{CDW}(x') \rangle &= \langle \Delta_{dimer}(x)\Delta_{dimer}(x') \rangle \\ &\sim |x-x'|^{-K_c}. \end{aligned} \quad (56)$$

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 $\langle \varphi_c \rangle = \sqrt{\pi/8K_c}$. The spin sector is gapped with $\langle \varphi_s \rangle = 0$. Using Eqs. (45)–(50) one obtains a LRO CDW in the ground state

$$\langle \Delta_{CDW}(x)\Delta_{CDW}(x') \rangle \sim \text{const}. \quad (57)$$

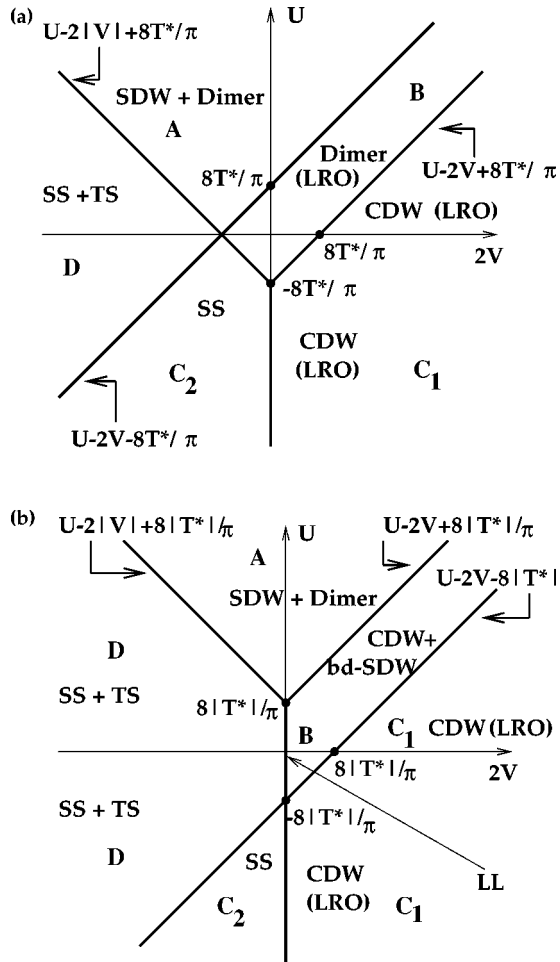


FIG. 3. Phase diagram of the model Hamiltonian Eq. (2) for the case of a half-filled band and (a) $T^* > 0$, (b) $T^* < 0$.

In the case of a repulsive nn interaction ($V > 0$), the effect of $T^* > 0$ is to split the SDW to CDW transition at $U = 2V$ into two parts substituting a metallic phase along the $U = 2V$ line by the LRO dimerized phase for $|U - 2V| < 8T^*/\pi$.

Sector C_2 : $U < -|2V + 8T^*/\pi|$ and $V < 0$. Here, a gap exists in the spin-excitation spectrum, the spin field is ordered with $\langle \varphi_s \rangle = 0$. The charge excitation spectrum is gapless and the fixed-point value of the parameter $K_c < 1$. The SS instability is the dominating one. At $U = 2V + 8T^*/\pi$ the spin gap closes. Triplet superconductivity is no longer suppressed, and $K_s = 1$, $K_c > 1$.

Sector D: $2V + 8T^*/\pi < U < -2V - 8T^*/\pi$. In this sector the system shows the properties of the LL metal with dominating superconducting instabilities

$$\langle \Delta_{SS}(x) \Delta_{SS}(x') \rangle = \langle \Delta_{TS}(x) \Delta_{TS}(x') \rangle \sim |x - x'|^{-1-1/K_c}. \quad (58)$$

Finally, we analyze the case $T^* < 0$ [see Fig. 3(b)]. The phase diagram once again consists of five different sectors.

Sectors A, C_1 , C_2 , and D are identical to the corresponding sectors for the $T^* > 0$ case. Particular is sector B: $|U - 2V| < 8|T^*|/\pi$ and $V > 0$. In this sector, the spin spectrum is gapless while the charge excitation spectrum is mas-

sive and the vacuum expectation value of the ordered charge field is $\langle \varphi_c \rangle = \sqrt{\pi/8K_c}$. Using Eqs. (45)–(50) one obtains in this sector an insulating phase with dominating CDW and bd-SDW instabilities showing a power-law decay at large distances

$$\begin{aligned} \langle \Delta_{CDW}(x) \Delta_{CDW}(x') \rangle \\ = \langle \Delta_{bd-SDW}(x) \Delta_{bd-SDW}(x') \rangle \sim |x - x'|^{-1} \end{aligned} \quad (59)$$

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 $T^* \rightarrow 0$ the sector with new phases shrinks to the line $U = 2V$ and the ground state phase diagram of the extended Hubbard model^{40–43} is recovered.

For $V = 0$ and $T^* < 0$, the SDW insulator-metal transition at $U = U_c = 8|T^*|/\pi$ is in qualitative agreement with results of numerical studies.³⁵ 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 $U = 2V + 8|T^*|/\pi$. There is no superconductivity for $V > 0$ in the weak-coupling phase diagram.

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.^{40,43}

However, in the case of strong CH interaction, numerical studies of the model (2) with ‘‘attractive’’ three-body interaction^{28,30,31,35} as well as exact results obtained at $T^* = 0$, $|t^*| = t$ (Refs. 18–21) show strong tendency towards superconducting ordering in the ground state. This discrepancy between the weak-coupling phase diagram and properties of the system in the case of strong CH interaction *indicate the presence of an additional phase transition with increasing correlated hopping coupling*. As far as all marginally relevant terms are incorporated within the continuum-limit approach, *this transition has to be charac-*

terized by a critical value of the coupling constant. Moreover, the exact solutions show local-pair (doublon) superconductivity, hence the transition seems to be completely determined by the finite bandwidth effects and therefore could not be traced within infinite band (continuum-limit) approach. In analogy with the pair-hopping model, where the transition into the local-pair superconducting state is due to the level-crossing phenomenon,⁵¹ one may assume a similar scenario for transition in the CH model as well. Density ma-

trix renormalization-group studies of sufficiently long chains will be very interesting to shed light on this question.

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