

## Triplet superconductivity in quasi-one-dimensional systems

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We study a Hubbard Hamiltonian, including a quite general nearest-neighbor interaction, parametrized by repulsion  $V$ , exchange interactions  $J_z, J_\perp$ , bond-charge interaction  $X$ , and hopping of pairs  $W$ . The case of correlated hopping, in which the hopping between nearest neighbors depends upon the occupation of the two sites involved, is also described by the model for sufficiently weak interactions. We study the model in one dimension with usual continuum-limit field theory techniques, and determine the phase diagram. For arbitrary filling, we find a very simple necessary condition for the existence of dominant triplet superconducting correlations at large distance in the spin SU(2) symmetric case:  $4V+J<0$ . In the correlated-hopping model, the three-body interaction should be negative for positive  $V$ . We also compare the predictions of this weak-coupling treatment with numerical exact results for the correlated-hopping model obtained by diagonalizing small chains and using a Berry phase to determine the opening of the spin gap. [S0163-1829(99)01046-2]

### I. INTRODUCTION

In the last years, the study of extensions of the usual Hubbard model has, among others, two important motivations. First, to explain many features of the rich diagram observed in the quasi-one-dimensional organic compounds (TMTSF)<sub>2</sub>X (where TMTSF means tetramethyltetraselenafulvalene and X represents, PF<sub>6</sub>, ClO<sub>4</sub> or other complex), other interactions must be considered in the model Hamiltonian, in addition to the on-site Coulomb repulsion.<sup>1-4</sup> Second, consensus increases about the fact that the usual Hubbard Hamiltonian<sup>5</sup> does not seem to define the minimal model for the superconducting cuprates, while additional terms might explain the physics of the superconducting phase of these materials.<sup>6</sup> The proximity between the spin density wave (SDW) and the superconducting phases observed in the phase diagrams of both kind of systems has been many times pointed out as a remarkable fact.<sup>1,2</sup> The symmetry of the order parameter is, however, different for both systems. While it has been observed to be  $d_{x^2-y^2}$  for the case of the cuprates,<sup>7</sup> experimental evidence suggests that the observed superconductivity in (TMTSF)<sub>2</sub>ClO<sub>4</sub>, and (TMTSF)<sub>2</sub>PF<sub>6</sub> under pressure,<sup>8</sup> as well as in the layered compound Sr<sub>2</sub>RuO<sub>4</sub> (Ref. 9) is of triplet  $p$ -wave character. In this context, the extended Hubbard model with correlated hopping is particularly interesting, as it seems to provide a good scenario for the occurrence of both kinds of superconducting instabilities, as well as the SDW and charge density wave (CDW) ones, depending on the values of the parameters and the filling factor.<sup>6,10-12</sup>

The model is defined by the Hamiltonian

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle} n_i n_j - \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) \\ \times \{ t_{AA} (1 - n_{i\sigma}) (1 - n_{j\sigma}) + t_{BB} n_{i\sigma} n_{j\sigma} + t_{AB} [n_{i\sigma} (1 - n_{j\sigma}) \\ + n_{j\sigma} (1 - n_{i\sigma})] \}, \quad (1)$$

where  $\langle ij \rangle$  denotes nearest-neighbor sites. This model contains the one which Hirsch proposed to give rise to hole superconductivity.<sup>13</sup> In the context of the superconducting cuprates, Eq. (1) has been obtained as a one-band effective Hamiltonian when a low energy reduction of the extended three-band Hubbard Hamiltonian is performed. For realistic parameters of the three-band model, calculated hopping parameters satisfy the following relation:  $t_{AB} > (t_{AA} + t_{BB})/2$ .<sup>14-17</sup> In particular, in the limit in which the Cu-O hopping  $t_{pd}$  is much smaller than the charge-transfer energies,  $t_{AB}$  is of the order of  $t_{pd}$ , while  $t_{AA}$  and  $t_{BB}$  are of order  $t_{pd}^2$ .<sup>16</sup> In two dimensions (2D), mean-field calculations, including the effect of spin fluctuations, support the existence of a superconducting phase with  $d_{x^2-y^2}$  symmetry at finite doping, which is stabilized with the addition of a next-nearest neighbor hopping in the Hamiltonian.<sup>6</sup> While a realistic effective Hamiltonian for (TMTSF)<sub>2</sub>X has not been constructed so far, Eq. (1) contains the main terms, if only the ground state with zero, one, and two particles in the singlet sector of an adequately chosen cell are retained.<sup>15,18</sup>

Collecting the correlated hopping terms in one-, two-, and three-body terms, the Hamiltonian reads

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle} n_i n_j + \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) \\ \times [-t + t_2 (n_{i\sigma} + n_{j\sigma}) + t_3 n_{i\sigma} n_{j\sigma}], \quad (2)$$

where  $t = t_{AA}$ ,  $t_2 = t_{AA} - t_{AB}$ , and  $t_3 = 2t_{AB} - t_{AA} - t_{BB}$ . While two-body interactions are usual in many-particle problems, three-body interactions are more rare and introduce additional complications in most of the usual analytical many-body treatments. The appropriate mean-field reduction of the three-body term with parameter  $t_3$  to effective two-body ones can be performed using Wick's theorem and neglecting the resulting normal ordered three body term, with

the vacuum representing the optimum Slater determinant.<sup>19,20</sup> In 1D, we have verified that in the continuum limit (representing the fermionic fields in terms of bosonic ones), this procedure is equivalent to perform operator product expansions in the resulting Hamiltonian, keeping only relevant and marginal operators.<sup>12</sup> In other words, both approaches are equivalent in the weak-coupling limit. The ensuing two-body Hamiltonian reads<sup>17</sup>

$$\begin{aligned}
H^{\text{eff}} = & U \sum_i n_{i\uparrow} n_{i\downarrow} + V^{\text{eff}} \sum_{\langle ij \rangle} n_i n_j + \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) \\
& \times [t^{\text{eff}} + \Delta(n_{i\sigma} + n_{j\sigma})] - W \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} + \text{H.c.}) \\
& + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (3)
\end{aligned}$$

with

$$\begin{aligned}
t^{\text{eff}} = & t - t_3(3\tau^2 - \rho^2), \quad V^{\text{eff}} = V + t_3\tau, \\
W = & 2t_3\tau, \quad \Delta = t_2 + \rho t_3, \quad J = 4t_3\tau, \quad (4)
\end{aligned}$$

where  $\tau = \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$  and  $\rho = \langle n_{i\sigma} \rangle = n/2$ , with  $n$  being the number of particles per site. In 1D and the weak coupling limit:

$$\tau = \frac{1}{\pi} \int_0^{k_F} dk \cos k = \frac{\sin(\pi\rho)}{\pi}, \quad \rho = \frac{1}{\pi} \int_0^{k_F} dk = \frac{k_F}{\pi}. \quad (5)$$

The Hamiltonian (3), with arbitrary interactions  $t^{\text{eff}}, \Delta, W, J, U, V^{\text{eff}}$ , defines the most general model with nearest neighbor two-body interactions, which conserves charge and spin SU(2) symmetry. If in addition, the parameters are related by Eq. (4) with  $V=0$ ,  $\rho=1/2$  and arbitrary  $\tau$ , the model also has pseudospin SU(2) symmetry.<sup>21</sup> In the general case, we will also include the possibility of anisotropic exchange ( $J_z$  in one direction,  $J_\perp$  in the other two), breaking spin SU(2) symmetry. Equation (3) contains all the contributions up to nearest neighbors of the Coulomb interaction when written in the tight binding basis.<sup>22,23</sup> In this case, for weak screening of the interatomic repulsion, the relation  $U > V^{\text{eff}} > \Delta > W \sim J > 0$  has been derived, while smaller values of  $V$  are expected if the screening is efficient.<sup>22,23,25</sup> Arbitrary values of the different interactions could, however, be expected when dealing with effective models, derived from some multiband model, as it is the case of Eq. (1).

Several specific cases of the model Eq. (3) have been studied before using continuum limit field theory (CLFT).<sup>4,12,23,24,26</sup> In particular, the chain described by the correlated hopping model Eq. (1) was analyzed recently at half filling.<sup>12</sup> However, no definite conclusions regarding possible dominance of superconducting correlations at large distances were obtained, and the extension to other fillings remains open. An accurate phase diagram has also been obtained numerically using topological transitions.<sup>10</sup> Other works on models similar to Eqs. (1) and (2) are cited in Refs. 12,27.

In this paper, we study the phase diagram of  $H_{\text{eff}}$  (3) with generic parameters ( $t^{\text{eff}}, t_2^{\text{eff}}, W, J_z, J_\perp, V^{\text{eff}}$ ), in the weak-coupling regime, using the CLFT. The boundaries of the

region with dominant triplet superconducting correlations at large distances are given by simple analytical expressions. This region will be denoted TS phase in the following. As a further step, we obtain the phase diagram of the correlated Hamiltonian Eq. (1), for weak and strong interactions, by numerical diagonalization of finite rings. The opening of the spin gap is detected accurately using the novel singlet-triplet level crossing method, based on results of conformal field theory and renormalization group.<sup>28</sup> This method is equivalent to a topological transition which corresponds to a jump in a Berry phase.<sup>29</sup> The results of both approaches are compared and the conditions for the existence of the TS phase are discussed. We also analyze the other phases of the model, and discuss within which region of parameters, a superconducting instability with  $d_{x^2-y^2}$  symmetry could be expected in 2D. Section II describes the weak coupling results. Results of the exact diagonalization of Eq. (1) and comparison with the CLFT are presented in Sec. III. Section IV contains a discussion.

## II. CONTINUUM LIMIT FIELD THEORY

The CLFT, also called g-ology, is a weak coupling approach. The whole procedure has been explained in detail in many contributions.<sup>3,4,12,26,30,31</sup> We, thus, present here only a brief explanation of the steps followed. The basic assumption is that the interactions are small, in comparison with the Fermi energy. The non-interacting energy dispersion relation is linearized around the two Fermi points and the interactions in the momentum space are expressed in terms of four different scattering processes, which are labeled by coupling constants  $g_{i\parallel}$  ( $g_{i\perp}$ ) if they involve the same (opposite) spins.

To describe the low-energy physics of the problem, the fermion operators are decomposed as

$$c_{j\sigma} \rightarrow \exp(ik_F R_j) \Psi_{+,\sigma}(j) + \exp(-ik_F R_j) \Psi_{-,\sigma}(j), \quad (6)$$

where  $\Psi_{r,\sigma}(j)$ ,  $r = \pm$  describe left- and right-moving fermions. In the continuum limit  $a \rightarrow 0$ ,  $L \rightarrow \infty$ , with  $aL$  finite,  $a$  being the lattice constant and  $L$  the number of sites of the lattice, these operators scale as  $\Psi_{r,\sigma}(j) \rightarrow \sqrt{a} \Psi_{r,\sigma}(x=ja)$ . The Hamiltonian (3) can be written in terms of the continuum fields  $\Psi_{r,\sigma}(x)$ .

Using the same notation as Voit<sup>3,4</sup> and neglecting irrelevant operators, we obtain the following coefficients for the different scattering processes of the Hamiltonian Eq. (3):

$$\begin{aligned}
g_{1\parallel} = & \left( 2V^{\text{eff}} + \frac{J_z}{2} \right) \cos(2k_F a), \\
g_{2\parallel} = & g_{4\parallel} = V^{\text{eff}} + \frac{J_z}{4}, \quad g_{3\parallel} = 0, \\
g_{1\perp} = & U + \left( 2V^{\text{eff}} - \frac{J_z}{2} \right) \cos(2k_F a) - J_\perp - 2W + 8\Delta \cos(k_F a), \\
g_{2\perp} = & \frac{U}{2} + V^{\text{eff}} - \frac{J_z}{4} - \frac{J_\perp}{2} \cos(2k_F a) - W + 4\Delta \cos(k_F a),
\end{aligned}$$

$$g_{3\perp} = \delta_{n,1} \left( U - 2V^{\text{eff}} + \frac{J_z}{2} + J_{\perp} + 2W \right),$$

$$g_{4\perp} = \frac{U}{2} + V^{\text{eff}} - \frac{J_z}{4} - \frac{J_{\perp}}{2} - W \cos(2k_F a) + 4\Delta \cos(k_F a),$$
(7)

where  $\delta_{n,1}$  in the  $g_{3\perp}$  (Umklapp) coupling constant indicate that this scattering process is active only at half filling. The fermion fields  $\Psi_{r,\sigma}(x)$  can be written in terms of bosonic fields  $\phi_{\rho}$ ,  $\phi_{\sigma}$ , where  $\rho$ , ( $\sigma$ ) denotes charge (spin) degrees of freedom, by recourse to a bosonization identity<sup>3</sup> and the Hamiltonian can be expressed as

$$H^{\text{eff}} = H_{\rho} + H_{\sigma},$$
(8)

where  $H_{\nu}$ , ( $\nu = \rho, \sigma$ ) is a sine-Gordon Hamiltonian:

$$H_{\nu} = v_{\nu} \int dx \left\{ \frac{1}{2} [\Pi_{\nu}^2(x) + (\partial_x \phi_{\nu})^2] + \frac{m_{\nu}}{a^2} \cos(\sqrt{8\pi K_{\nu}} \phi_{\nu}) \right\},$$
(9)

where  $\Pi_{\nu}$  is the moment conjugate to  $\phi_{\nu}$ , and

$$v_{\nu} = \sqrt{(v_F^{\nu})^2 - \left( \frac{g_{\nu}}{2\pi} \right)^2}, \quad m_{\rho} = \frac{g_{3\perp}}{2\pi}, \quad m_{\sigma} = \frac{g_{1\perp}}{2\pi},$$

$$v_F^{\rho} = v_F + \frac{g_{4\parallel} + g_{4\perp}}{\pi}, \quad v_F^{\sigma} = v_F + \frac{g_{4\parallel} - g_{4\perp}}{\pi}$$

$$v_F = 2t_{\text{eff}} \sin\left(\frac{\pi n}{2}\right), \quad K_{\nu} = \sqrt{\frac{2\pi v_F^{\nu} + g_{\nu}}{2\pi v_F^{\nu} - g_{\nu}}},$$
(10)

with

$$g_{\rho} = 2g_{1\parallel} - g_{2\parallel} - g_{2\perp}, \quad g_{\sigma} = 2g_{1\parallel} - g_{2\parallel} + g_{2\perp}. \quad (11)$$

The physics of the sine-Gordon Hamiltonian is well known from renormalization group.<sup>3,30,31</sup> At half-filling, for  $|g_{3\perp}| \leq g_{\rho}$  the charge sector renormalizes to the Tomonaga-Luttinger fixed point, where charge excitations are gapless. Away from half-filling, charge excitations are gapless, except for commensurate fillings  $n = p/q$  and strong repulsive interactions:<sup>32</sup> the system is insulating if  $K_{\rho} < 1/q^2$ . For example at quarter filling ( $n = 1/2$ ), the critical value of  $K_{\rho}$  is  $1/4$ .<sup>32,33</sup> In terms of the parameters of Eq. (3), the condition for Luttinger liquid behavior at half filling reduces to

$$2U + 4V^{\text{eff}} + 2J_{\perp} + J_z \leq 0 \quad \text{and} \quad 2V^{\text{eff}} \leq W. \quad (12)$$

For the particular case of the extended Hubbard model with correlated hopping (2), using Eqs. (4), (5), and (7), this condition reads

$$(U + 2V + 8t_3/\pi \leq 0 \quad \text{and} \quad V \leq 0) \quad (13)$$

in agreement with Ref. 12. In particular, for  $V > 0$  the system has always a charge gap at half filling.

Out of half filling, the Hamiltonian  $H_{\rho}$  [see Eqs. (9), (10), and (7)], reduces to a Gaussian model (except for higher order Umklapp processes which are relevant for commensurate fillings and  $K_{\rho} \leq 1/4$ , as mentioned above<sup>32,33</sup>). In this case,  $K_{\rho}$  is not renormalized and if  $K_{\rho} > 1$  superconducting

correlations dominate at large distances. From Eq. (10), this happens when  $g_{\rho} > 0$ . At half filling,  $K_{\rho}$  is renormalized, but the initial value [Eq. (10)] should be larger than one in order to reach a final value larger than one at the Gaussian point in the renormalization-group procedure. Thus, from Eqs. (5), (10), (7), and (11), a necessary condition for the dominance of superconducting correlations at large distances is obtained:

$$-U - 4V^{\text{eff}} + \left( 2V^{\text{eff}} + \frac{J_z}{2} + J_{\perp} \right) \cos(\pi n) + 2W - 8\Delta \cos(\pi n/2) > 0. \quad (14)$$

This condition is also sufficient away from half filling ( $n \neq 1$ ). The character of the dominant superconducting correlations at large distances (singlet or triplet) and simultaneously the opening of a spin gap is determined by  $H_{\sigma}$  [Eq. (9)] and the flow of its parameters under renormalization. In the spin SU(2) invariant case ( $J_z = J_{\perp}$ ),  $g_{\sigma} = g_{1\perp}$ . For negative  $g_{\sigma}$  a spin gap opens, the triplet superconducting (TS) correlations functions (CF) decay exponentially, while the singlet superconducting (SS) CF decay as  $d^{-1/K_{\rho}}$  with distance  $d$ . Instead, for positive  $g_{\sigma}$ ,  $K_{\sigma}$  renormalizes to 1, there is no spin gap, the TS CF decay as  $d^{-1-1/K_{\rho}} \ln^{1/2} d$  and dominate over the SS CF, which decay as  $d^{-1-1/K_{\rho}} \ln^{-3/2} d$ .<sup>3</sup> Thus, in the Tomonaga-Luttinger liquid phase with  $J_z = J_{\perp}$  and  $K_{\rho} > 1$ , using Eqs. (5),(7),(10),(11), one sees that TS CF dominate at large distances if and only if

$$U + \left( 2V^{\text{eff}} - \frac{J}{2} \right) \cos(\pi n) - J - 2W + 8\Delta \cos(\pi n/2) > 0. \quad (15)$$

If the model is not spin SU(2) invariant, TS CF dominate, decaying as  $d^{-1/K_{\rho} - 1/K_{\sigma}}$  when  $K_{\rho} > 1$  and  $g_{\sigma} > |g_{1\perp}|$ , which in turn implies that the renormalized  $K_{\sigma} > 1$ .

Adding Eqs. (14) and (15) a very simple necessary condition for the existence of the TS phase in the model Eq. (3) with  $J_z = J_{\perp}$  is obtained:

$$4V^{\text{eff}} + J < 0. \quad (16)$$

This result is consistent with theoretical analysis which relates triplet superconductivity with ferromagnetism.<sup>34</sup>

For the model with correlated hopping in the form of Eq. (2), using Eqs. (4),(5) the conditions (14),(15) take the form

$$-U + 2V[\cos(\pi n) - 2] + \frac{8}{\pi} t_3 \sin(\pi n/2) \cos(\pi n) - 8(t_2 + t_3 n/2) \cos(\pi n/2) > 0, \quad (17)$$

in order that superconducting CF dominate at large distances and

$$U + 2V \cos(\pi n) - \frac{8}{\pi} t_3 \sin(\pi n/2) + 8(t_2 + t_3 n/2) \cos(\pi n/2) > 0 \quad (18)$$

for the region in which the spin gap is closed. Adding both conditions leads to

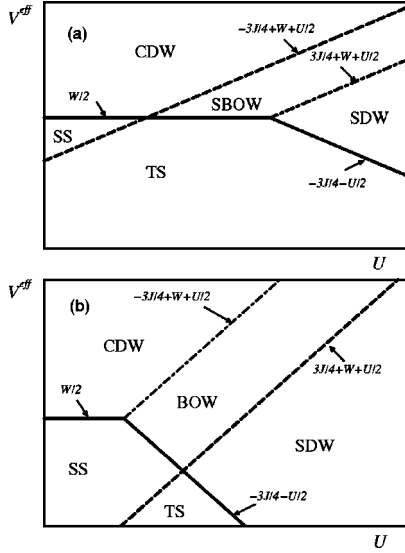


FIG. 1. Phase diagram of the general model Eq. (3) at half filling ( $n=1$ ) for  $J_{\perp}=J_z=J$ . (a)  $2W+J<0$ , (b)  $2W+J>0$ .

$$V + \frac{2}{\pi} t_3 \sin(\pi n/2) < 0, \quad (19)$$

as a necessary condition for the model to have a TS phase. In the extended Hubbard model ( $t_2=t_3=0$ ), Eqs. (17) and (18) imply that a TS phase can only exist for  $2/3 \leq n \leq 4/3$ .

In addition to the SS and TS CF, the phase diagram at half filling is determined by the CF at large distances of the following order parameters for charge density wave (CDW), spin density wave (SDW), bond ordering wave (BOW), and spin bond ordering wave (SBOW) order<sup>3,12</sup>

$$\begin{aligned} O_{\text{CDW}} &= \sum_{i\sigma} (-1)^i n_{i\sigma} \sim \cos(\sqrt{2\pi K_{\rho}} \phi_{\rho}) \cos(\sqrt{2\pi K_{\sigma}} \phi_{\sigma}), \\ O_{\text{SDW}} &= \sum_{i\sigma} (-1)^i \sigma n_{i\sigma} \sim \sin(\sqrt{2\pi K_{\rho}} \phi_{\rho}) \sin(\sqrt{2\pi K_{\sigma}} \phi_{\sigma}), \\ O_{\text{BOW}} &= \sum_{i\sigma} (c_{i+1\sigma}^{\dagger} c_{i\sigma} + \text{H.c.}) \\ &\sim \sin(\sqrt{2\pi K_{\rho}} \phi_{\rho}) \cos(\sqrt{2\pi K_{\sigma}} \phi_{\sigma}), \\ O_{\text{SBOW}} &= \sum_{i\sigma} \sigma (c_{i+1\sigma}^{\dagger} c_{i\sigma} + \text{H.c.}) \\ &\sim \cos(\sqrt{2\pi K_{\rho}} \phi_{\rho}) \sin(\sqrt{2\pi K_{\sigma}} \phi_{\sigma}), \end{aligned} \quad (20)$$

The opening of the spin gap is accompanied by the ordering of  $\phi_s$  with expectation value  $\langle \phi_s \rangle = 0$ . When the charge gap is closed, except for the particular case  $g_{\rho} = |g_{3\perp}|$  for which  $K_{\rho}$  renormalizes to 1,  $g_{\rho}$  renormalizes to a positive value and  $K_{\rho} > 1$  at the fixed point. Then, as discussed above, TS (SS) CF dominate at large distances if the spin gap is closed (open). Instead, when the charge gap opens ( $|g_{3\perp}| > g_{\rho}$ ),  $\phi_{\rho}$  orders with expectation value  $\langle \phi_{\rho} \rangle = 0$  [ $\langle \phi_{\rho} \rangle = \sqrt{\pi/(8K_{\rho})}$ ] for negative (positive)  $g_{3\perp}$ . If the spin gap is positive, this implies CDW (BOW) order, while if the spin gap is closed the dominant CF are the SBOW (SDW) ones.<sup>3,4,12</sup> These

considerations lead to the phase diagram shown in Fig. 1 for the general model Eq. (3) at half filling in the isotropic case  $J_{\perp}=J_z=J$ . For  $W=J=0$ , the model reduces to the extended Hubbard model studied previously,<sup>4,24,35</sup> and no BOW or SBOW phases appear. For large positive  $U$  the leading power-law decay of the SDW, CDW, and BOW CF is  $1/d$ , but the logarithmic correction of the former ( $\ln^{1/2} d$ ), makes the SDW the dominant CF at large distances.<sup>4</sup> The combination of parameters which control the existence of the BOW and SBOW phases is  $2W+J$ . The BOW (BSDW) CF dominate in a certain region of  $U$  and  $V$  if and only if  $2W+J > 0$  ( $2W+J < 0$ ), particularly for large  $U$  near the line  $V = U/2 - W - J/4$  at which the spin gap opens.

### III. NUMERICAL RESULTS

In this section we calculate the phase diagram of the correlated hopping model Eq. (1) by exact diagonalization of finite rings, and compare the results with those of the previous section. We concentrate on the electron-hole symmetric case and set  $t_{AA}=t_{BB}=1$ . Numerical<sup>10</sup> and CLFT (Ref. 12) results for one particle per site ( $n=1$ ) have been done recently. We have concentrated on two other densities:  $n=1/2$  (quarter filling) and  $n=2/3$ . The boundary of the superconducting phase was determined from the equation  $K_{\rho}=1$ , with  $K_{\rho}$  calculated from the expression

$$K_{\rho} = \sqrt{\pi \kappa D_{\rho}}/2, \quad (21)$$

where the Drude weight  $D_{\rho}$  and the compressibility  $\kappa$  were obtained extrapolating to the thermodynamic limit numerical results (obtained in the usual way<sup>36</sup>) using a polynomial in  $1/L$ , where  $L$  is the length of the ring. For  $n=1/2$ , we have used rings with  $L=8, 12$ , and  $16$ , and for  $n=2/3$  the lengths used were  $L=6$  and  $12$ . We have also calculated  $K_{\rho}$  using other two expressions which involve  $v_{\rho}$ , the central charge and charge and spin gaps,<sup>36</sup> to check for consistency and finite-size effects. The latter are in general very small, except for specific cases mentioned below. The opening of the spin gap was determined from the crossing of the levels of lowest energy in the sectors with total spin  $S=0$  and  $S=1$  for periodic (antiperiodic) boundary conditions if  $N/2$  is even (odd), where  $N$  is the number of particles in the system.<sup>28</sup> This method is based on results of conformal field theory and renormalization group, which show in addition that at the crossing point, the finite size corrections of these excitation energies per site go as  $1/L^2$ , without logarithmic corrections. This allows a very accurate determination of the parameters for which the spin gap opens using finite-size scaling. This level crossing has also a topological significance, since at this point, the spin Berry phase, which can only take two values:  $0$  or  $\pi \pmod{2\pi}$  jumps in  $(\pi)$  at the transition.<sup>29</sup>

In Fig. 2, we show the evolution with doping of the phase diagram for  $V=0$ . As soon as the density decreases below  $n=1$ , the Umklapp processes become irrelevant and according to the CLFT, the degeneracy of TS and SBOW CF on one phase and the SS and CDW on the other<sup>10,12</sup> is broken in favor of the superconducting CF, since  $K_{\rho}$  becomes larger than one. As doping increases, the SDW phase advances over the TS phase and at quarter filling ( $n=1/2$ ) the TS phase lies entirely within the region of negative  $U$ . Instead the SS phase advances rapidly over the BOW (or dimer or-

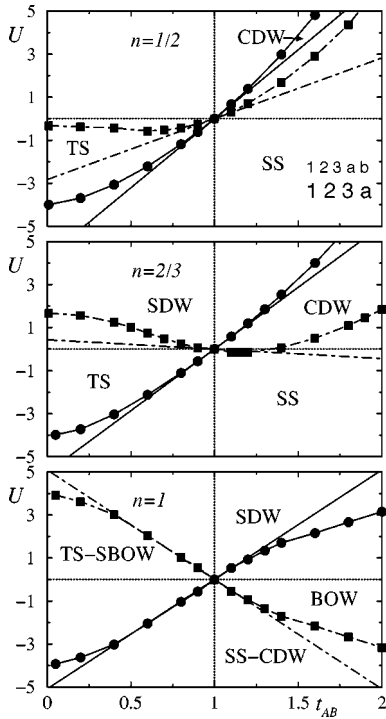


FIG. 2. Phase diagram of the correlated hopping model Eq. (1) for  $V=0$  and several densities indicated at the top left of each figure. Solid squares indicate values of  $U$  and  $t_{AB}$  for which  $K_\rho = 1$ . The straight line  $K_\rho = 1$  according to the CLFT [Eq. (17) with  $t_2 = 1 - t_{AB}$ ,  $t_3 = -2t_2$ ] is shown dot dashed. Solid circles are points at which the spin gap closes. The corresponding results according to the CLFT [Eq. (18)] are represented by the full straight line.

dered) phase at half filling. The agreement of the predictions of the singlet-triplet level crossing method for detecting the opening of the spin gap with the CLFT results is excellent at weak coupling ( $|t_{AB} - 1| < 0.1$ ), which confirms the accuracy of the method. The numerical results for the points at which  $K_\rho = 1$  also agree very well with the weak coupling results for  $n = 1/2$ . For  $n = 2/3$ , for which only two points ( $L = 6$  and  $L = 12$ ) were used in the finite-size scaling, and  $K_\rho$  varies very slowly with the parameters near the noninteracting limit, the numerical points in the weak coupling limit are not accurate enough. However, these points are also consistent with the CLFT results.

It is remarkable that for  $n = 1$ , the CLFT results are quantitatively valid even at intermediate coupling. However, out of half filling and weak coupling, the CLFT overestimates the region in which the spin gap vanishes, and clearly underestimate the extension of the superconducting phases.

In Fig. 3 we show the effect of  $V$  on the phase diagram for  $n = 2/3$ . We have chosen this density because a TS phase exists for positive  $U$  if  $t_{AB} < 1$ . For  $t_{AB} < 0.4$  the results are affected by large finite size effects, perhaps because of the proximity of phase separation (PS), and we were unable to obtain reliable results. For  $0.4 \leq t_{AB} < 1$ , increasing  $V$ , from zero, the line of  $K_\rho = 1$  is crossed first and then at larger  $V$  a spin gap opens, in qualitative agreement with the CLFT results. However, we obtain that the spin gap opens also when  $V$  is decreased taking negative values. This crossing is out of the reach of the CLFT. As  $V$  is further decreased one expects

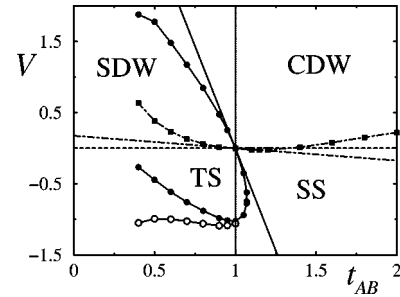


FIG. 3. Same as Fig. 2 for  $U=0$  and  $n=2/3$ . The open circles are points which correspond to the singlet-triplet crossing for  $L = 12$  and deviate substantially from the extrapolated results that indicate the opening of a spin gap.

PS. For  $t_{AB} < 0.9$  our results for the opening of the spin gap at negative  $V$  are affected by large finite size effects (reflected by the difference between the values of  $V$  indicated with solid and open circles in Fig. 3). This is probably caused by the proximity to PS. The numerical investigation of PS is very delicate<sup>37</sup> and is beyond the scope of this work.

#### IV. DISCUSSION

We have studied the phase diagram of a Hubbard model Eq. (3) in the weak coupling limit, generalizing previous studies which use the continuum limit field theory. The model includes the most general form of nearest-neighbor two-body interactions which conserves charge and spin. The phase diagram is very rich, and six different phases can appear, according to the dominant correlation functions at large distances (see Fig. 1). In particular, in the isotropic case, if there is a nearest-neighbor attraction ( $V < 0$ ) or ferromagnetic exchange ( $J < 0$ ) a phase with dominant triplet superconducting correlations (TS phase) can exist. Specifically  $4V + J < 0$  is a necessary condition for the existence of the TS phase. Work on weakly coupled chains using perturbation theory suggests that small interchain hopping stabilizes a 3D long-range order with finite critical temperature, which corresponds to the dominant correlations at large distances in the purely 1D case.<sup>39</sup> Thus, we expect that our results can be applied to real quasi-one-dimensional materials, which can be described by an effective Hamiltonian such as Eq. (1) or (3). Since in real materials  $V$  is expected to be repulsive, an efficient screening of the interatomic repulsions and effective ferromagnetic exchange (such as that present in one-dimensional cuprates containing edge-sharing  $\text{CuO}_4$  units<sup>38</sup>) would be necessary conditions for the existence of triplet superconductivity. It has been proposed that in some ideal limit, ferromagnetism and triplet superconductivity might be related by symmetry operations of the group  $\text{SO}(5)$ .<sup>34</sup>

For weak coupling, the general model Eq. (3), with parameters satisfying the relations Eq. (4) describes the correlated hopping model Eq. (1). For this model to display a TS phase in the weak coupling limit, it is necessary that  $V + (2/\pi)(2t_{AB} - t_{AA} - t_{BB})\sin(\pi n/2) < 0$ . We have studied this model beyond the weak coupling regime by numerical diagonalization of finite rings. In spite of the fact that the size of the studied systems is small, the results agree very well with those obtained with the field theory in the weak coupling regime. In particular, the accuracy of determining

the gap by the method of the crossing of singlet and triplet excitations<sup>28</sup> (which in turn is equivalent to a topological transition in the spin Berry phase<sup>29</sup>) is confirmed. For values of the correlated hopping which are outside the reach of the field theory, the regions of dominating superconducting correlations at large distances extend beyond the predictions of the weak coupling treatment.

There are other physical phenomena which are outside the scope of the field theoretical treatment we followed. One of them is the opening of the spin gap for  $t_{AB} < 1$  and negative  $V$  found in our numerical calculations (see Fig. 3). Another one is phase separation. In addition, for very small  $t_{AB}$  ( $t_{AB} = 0.2$ ), there is numerical evidence of peaks at incommensurate wave vectors in charge-charge and spin-spin correlation functions at half filling.<sup>11</sup> These can be qualitatively understood using the formalism of the exact solution for  $t_{AB} = 0$ :<sup>21</sup> roughly, the doubly occupied sites are represented by effective bosons and the singly occupied sites by effective fermions. The Fermi wave vector of these effective fermions depends on  $U$  and hence, it is in general different from the noninteracting Fermi wave vector. Unfortunately, a quantitative analytical calculation of these correlation functions for small  $t_{AB} \neq 0$ , is very difficult due to the huge degeneracy for  $t_{AB} = 0$ . On the level of the field theory, one might speculate that irrelevant operators, which we have neglected, become important at large couplings in an adequate renormalization group treatment and lead to incommensurabilities. In addition to the TS phase, the region of singlet superconductivity (SS) for  $t_{AB} > 1$  and  $U > 0$  (see Fig. 2) is particularly interesting. In the case  $t_3 = 2t_{AB} - t_{AA} - t_{BB} = 0$ , SS has been proposed and found in a mean-field treatment by Hirsch as a model for hole superconductivity,<sup>13</sup> and confirmed by other numerical and analytical calculations.<sup>12,26,27,36</sup> However, the case we studied numeri-

cally in Sec. III is electron-hole symmetric and  $t_3$  plays an important role. It is also essential in 2D to give rise to  $d_{x^2-y^2}$ -wave superconductivity.<sup>6</sup> In the limit in which  $t_{AB}$  is much larger than all other energy scales of the system, at half filling, a reasonable approximation to the ground state is obtained splitting the ring into consecutive dimers, and solving the Hamiltonian in each dimer. Including the hopping between dimers in second-order perturbation theory leads to an energy which is above the energy calculated with density-matrix renormalization group by 1.6%.<sup>10</sup> This suggests a picture in which the system is composed of dimers, which behave as hard core bosons, being frozen at half filling (leading to a dimerized phase with long range order, BOW in Fig. 2) but which acquire mobility out of half filling, giving rise to dominant SS correlations. If this image can be extended to 2D, we expect some kind of short range resonance-valence bond ground state at half filling, since dimers can be ordered in many different ways, and SS of  $s$ - or  $d_{x^2-y^2}$ -wave symmetry would naturally arise as the system is doped. The favored symmetry depends on the topology of the Fermi surface. According to mean-field calculations and including spin fluctuations, the  $d_{x^2-y^2}$ -wave symmetry is favored for moderate doping if a negative next-nearest-neighbor hopping is included in the model.<sup>6</sup> We are presently investigating this possibility by numerical diagonalization.

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