Superconducting ground state in a model with bond-charge interaction

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An electronic Hubbard-type model with bond-charge interaction and on-site repulsion U is studied in one and two dimensions. Evidence is provided in favor of superconductivity, without phase separation, for $U < U_c(n)$, although no explicit attraction between particles is present in the Hamiltonian. The presence of a bound state for two particles in vacuum for $D = 1$ and 2 (but not for $D = 3$) suggests that, at low density and low dimensionality, superconductivity is due to condensation of preexistent pairs (dimers). The one-dimensional (1D) phase diagram is studied analytically as well as numerically and shows a transition between a Luttinger liquid and a strong-coupling phase with diverging superconducting susceptibility. Estimates of critical exponents are given at low density and at quarter filling for several values of the parameters. The 2D model at quarter filling is analyzed by Lanczos diagonalization on a 4×4 cluster. The numerical results are consistent with the phase diagram obtained by BCS mean-field theory and is qualitatively similar to the 1D case: a ground state with spin gap and off-diagonal long-range order at $U < U_c(n)$; and a Fermi liquid above U_c with no sign of phase separation.

I. INTRODUCTION

The discovery of high-T_c superconducting materials has revived interest in the physics of strongly correlated electronic systems and much work has been devoted to the search for superconductivity in Hubbard-type models. It soon became clear that superconductivity in purely electronic one-dimensional (1D) and 2D systems can be induced by direct (*diagonal*) interactions, as in the extended Hubbard model (with $V < 0$) or in the t-J model at sufficiently large J. This mechanism is rather insensitive to dimensionality and, although off-diagonal long-range order cannot be achieved in one dimension, clear signals of a superconducting instability are present also in 1D models.[1,2] A serious drawback of this type of mechanism is the presence of (at least) another instability leading to phase separation, which occurs just nearby the superconducting region in systems with nonzero-range interactions (like the negative U Hubbard model). A very unlikely fine-tuning of the parameters in the Hamiltonian is needed to obtain superconductivity without phase separation.[3] The physical reason for the proximity of the two instabilities can be traced back to the essentially *classical* (density-density or spin-spin) character of the interaction which generates superconductivity. If this interaction becomes sufficiently strong, it overcomes the kinetic energy term and favors the state which minimizes the potential energy, giving rise to phase separation.

A different type of *nonclassical* interaction leading to superconductivity without other instabilities has been advocated by Hirsch and Marsiglio in a series of papers[4–6] in order to explain superconductivity in high-T_c oxides. The key additional term is a *bond-charge* interaction, besides the usual Hubbard U repulsive term due to the always present (screened) Coulomb potential. A simple, intuitive, interpretation of this interaction is a *density-dependent hopping* term which, say, enhances hopping when (at least) one of the two orbitals involved in the hopping process is occupied by another electron. Such a term emerges rather naturally in the construction of a tight-binding Hamiltonian[7,8] and can naturally be thought of as the result of a trace over additional degrees of freedom of either electronic[9] or of different physical origin.[10] Exact solutions for special choices of the parameters have also been recently obtained in similar 1D models.[11–13]

In this paper we will take such a bond-charge model as an effective electronic model without entering into a discussion about the physical origin of the interaction. The emphasis of our investigation will be on the properties of these systems and on the resulting zero-temperature phase diagram both in one and two dimensions. In particular, we will show, by use of analytical as well as numerical techniques, that in a wide parameter region the model has a superconducting ground state. The character of the Cooper pair changes with density, at fixed interaction strength, going from real space dimers at low density to less strongly bound pairs when the density is increased. The analysis of the model can be made fully quantitative in 1D because of the extremely powerful techniques available in one-dimensional systems: bosonization, conformal field theory, and weak-coupling renormalization group which can be successfully supplemented by numerical methods. In 2D, the low-density part of the phase diagram can be obtained exactly and numerical diagonalizations at quarter filling support a mean-field approximation.

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The paper is organized as follows: In Secs. II and III we introduce the model, providing the exact solution for a few particles in a vacuum. In Secs. IV and V we calculate the one-dimensional correlation exponents both in the zero-density limit, starting from the two- and four-particle solution, and at quarter filling by a finite-size scaling analysis. Section VI is dedicated to the BCS solution of the model in any dimension. Finally Sec. VII is devoted to a discussion of the ground-state phase diagram both in one and in two dimensions.

II. TWO-PARTICLE PROBLEM

The Hamiltonian we are going to analyze is that of a Hubbard model with correlated hopping and reads

$$H = -\sum_{\langle rr' \rangle} \sum_{\sigma} (c^{\dagger}_{r\sigma} c_{r'\sigma} + \text{H.c.}) \left[t - \gamma \left(n_{r'-\sigma} + n_{r-\sigma} \right) + \beta\, n_{r'-\sigma}\, n_{r-\sigma} \right] + U \sum_{r} n_{r\uparrow}\, n_{r\downarrow}. \tag{1}$$

The interaction term includes the on-site Coulomb repulsion U and the bond-charge interactions γ and β, which describe an enhanced hopping amplitude for particles in doubly occupied sites. The number operator for electrons of spin σ on a site r is denoted by $n_{r\sigma} = c^{\dagger}_{r\sigma} c_{r\sigma}$

Hamiltonian (1) coincides with that derived by Simon and Aligia[9] as an effective one-band model resulting from tracing out the degrees of freedom associated with the oxygen electronic band in cuprates. The model is rather general but we will mainly focus on two simple parameter choices: (i) $\beta = 0$, i.e., keeping only terms with at most four fermion operators, and (ii) $\beta = \gamma^2/t$ where the interaction acquires a particular symmetrical form and can be easily interpreted as a tight-binding model with a density-dependent hopping amplitude:

$$t \to t \left(1 - \frac{\gamma}{t} n_{r-\sigma} \right) \left(1 - \frac{\gamma}{t} n_{r'-\sigma} \right). \tag{2}$$

We first address the problem of a few particles in a vacuum by reviewing the exact solution of two-body problem in arbitrary dimension which was investigated by Marsiglio and Hirsch.[14] Let us consider two electrons: In this case the β term in the Hamiltonian is ineffective and can be dropped. A generic state in the Hilbert space with a total z component of the spin equal to zero can be written as

$$|\Psi\rangle = \sum_{r,r'} \psi(r,r')\, c^{\dagger}_{r\uparrow}\, c^{\dagger}_{r'\downarrow}\, |0\rangle\,, \tag{3}$$

where the vacuum $|0\rangle$ is the state without electrons.

The Schrödinger equation is easily solved in momentum space where the wave function of the singlet spectrum has the form

$$\psi_k = A + \frac{B}{E - \epsilon_k - \epsilon_{P-k}}. \tag{4}$$

P is the total momentum of the state, ϵ_k is the tight-binding dispersion of the free-electron problem ($\epsilon_k = -2t \sum_{\alpha} \cos k_{\alpha}$), and the two constants A and B are related to the value of the wave function at $r = 0$ and at nearest neighbors. By imposing the self-consistency condition, we obtain the eigenvalue equation for the energy E in an arbitrary spatial dimension:

$$\frac{1}{N} \sum_{k} \frac{1}{E - \epsilon_k - \epsilon_{P-k}} = \frac{(\gamma - t)^2}{E\,\gamma\,(\gamma - 2\,t) + U\,t^2}. \tag{5}$$

It is worth mentioning that the eigenvalue equation is formally identical to that of the Hubbard model: In this case, the right-hand side of Eq. (5) would simply read $1/U_{\text{eff}}$, allowing for a bound state only if $U_{\text{eff}} < 0$. Instead Eq. (5) has a bound state for $\gamma < 0$ both in one and two dimensions, at every value of the total momentum P and even for repulsive $U > 0$, up to

$$U_c = 4\,D\,\gamma \left(\frac{\gamma}{t} - 2 \right) \tag{6}$$

for $D \leq 2$, where D is the space dimensionality. So a finite, positive $U > U_c$ is needed in order to destroy the bound pair. Remarkably, the rather strong attraction responsible for this binding is generated by the bond-charge interaction alone. The binding mechanism involves a gain in kinetic energy when two particles are at a nearest-neighbor distance. This interpretation is supported by the form of the wave function which is peaked not just on site but also at the nearest neighbors, while decreasing exponentially elsewhere. The critical U_c increases in going from one to two dimensions because of the enhanced efficiency of the bond-charge interaction which grows when the number of nearest neighbors increases. The absolute ground state is always in the $P = 0$ sector and the presence of a bound state for any total momentum P is easily interpreted as describing a coherent motion of the bound pair. At larger values of U double occupancies are suppressed, inhibiting the mechanism leading to binding: The pair breaks and the low-energy spectrum is continuous.

III. FEW-PARTICLE BOUND STATES IN $D = 1$

For two particles in $D = 1$, the bound-state solution can be worked out analytically, leading, in the thermodynamic limit, to the ground-state energy

$$E_b(P) = \frac{U\gamma(\gamma - 2t) - (\gamma - t)^2 \sqrt{U^2 + 8\,(1 + \cos P)(t^2 - 4\gamma t + 2\gamma^2)}}{t^2 - 4\gamma t + 2\gamma^2} \tag{7}$$

and to an exponentially bound pair wave function which in real space reads

$$\psi(r) = \psi(0)\left[\left(1-\frac{\gamma}{t}\right)e^{-\lambda r}+\frac{\gamma}{t}\delta_{r,0}\right] \quad (8)$$

for $P=0$. Here, the size of the pair $1/\lambda$ is a function of the parameters γ and U and diverges along the critical line (6):

$$\lambda = -\ln\left[\frac{t}{4}\,\frac{U+\sqrt{U^2+16\,(t^2-4\gamma t+2\gamma^2)}}{t^2-4\gamma t+2\gamma^2}\right]. \quad (9)$$

As previously discussed, an attraction between pairs in a vacuum may lead either to superconductivity or to phase separation according to the form of the *residual interaction* once the pair is formed. The best way to investigate the sign of this residual interaction is via a direct calculation of the ground-state energy of a system of four particles. This problem becomes particularly simple in the $U\to-\infty$ limit because our model maps onto a standard negative U Hubbard model with effective hopping $t'=t-\gamma$ and the binding energy of the four-particle system $\Delta E = E(4)-2E(2)$ can be explicitly evaluated to order $1/U$:

$$\Delta E = E(4)-2\,E(2) = \frac{(\gamma-t)^2}{|U|}\,\frac{4\pi^2}{L^2}+O\left(\frac{1}{U^2}\right). \quad (10)$$

Note that the binding energy is positive and vanishes in the thermodynamic limit. This provides a strong indication for the absence of bound states involving more than two particles and suggests that the model, in the low-density regime, behaves as a dilute gas of bound pairs which are characterized by a weak repulsive residual interaction. These composite particles (*dimers*) are characterized by their effective mass which can be evaluated through the momentum dependence of the two-particle ground-state energy $E_b(P)$ (7). At large negative U and (small) total momentum P, $E_b(P)$ can be expanded as[15] $E(P)=E_0+t_{\rm eff}\,P^2$ where the dimer hopping amplitude is $t_{\rm eff}=-2\,(\gamma-t)^2/U$. This result is entirely compatible with a picture of dimers behaving as a gas of hard core bosons with effective hopping amplitude $t_{\rm eff}$. In fact, the representation in terms of free hard core bosons would imply a zero-point kinetic energy $t_{\rm eff}\,2\pi^2/L^2$ which agrees with the four-particle perturbative result (10) via the definition of $t_{\rm eff}$. This fact gives us confidence in the picture of the low-density regime as a dimer gas and allows us to extend the definition of the effective hopping amplitude for dimers by use of Eq. (7) at arbitrary $U<U_c$:

$$t_{\rm eff} = \frac{2\,(t-\gamma)^2}{\sqrt{U^2+16\,(t^2-4\,\gamma\,t+2\gamma^2)}}. \quad (11)$$

In order to provide a check on expression (11) and to confirm the superfluid dimer picture, we can solve the four-particle problem at $U=0$ by exact diagonalization of the Hamiltonian (1). The zero-point kinetic energy of the four particles ΔE is numerically evaluated in 1D rings as

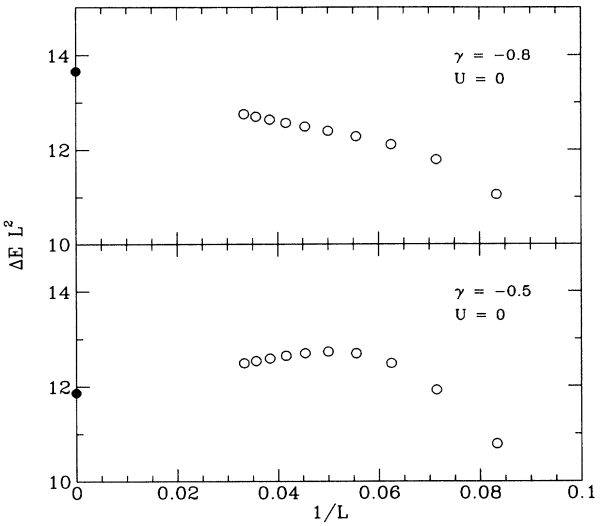

FIG. 1. Size scaling of the ground-state energy of the Hamiltonian in Eq. (1) with $U=0$ and four electrons for two different values of the parameter γ. $\Delta E = E(4,L)-2E(2,\infty)$ where $E(N,L)$ is the ground-state energy of N electrons in an L-site ring in units of t. The solid circle is the theoretical value for two hard core bosons in the infinite lattice with $t_{\rm eff}$ given by Eq. (11).

$$\Delta E = E(4,L)-2\,E(2,\infty) = \frac{2\,\pi^2}{L^2}\,t_{\rm eff}. \quad (12)$$

The finite-size scaling of the numerical results is shown in Fig. 1 for two different values of γ, and $\beta=\gamma^2/t$ proves that ΔE is positive and vanishes in the thermodynamic limit (i.e., the four particles do not form a bound state). Moreover, the asymptotic behavior of ΔE as $L\to\infty$ agrees with the theoretical value obtained via Eq. (11), also shown in the figure.

In conclusion we can state that the model is stable against phase separation. The system behaves as a dilute gas of dimers, which follow boson statistics and can be treated as hard core particles. Therefore it is quite plausible that, at least at low density, the ground state is a superconductor via Bose condensation of preexistent pairs. This result is rather robust against the presence of Hubbard repulsion U and a remarkably large value of $U>0$ is needed to break these pairs. Of course in 1D the quantum fluctuations prevent actual Bose condensation and only a ground state with power law superconductive correlations and diverging susceptibility is expected.

IV. CORRELATION EXPONENTS IN 1D: ZERO-DENSITY LIMIT

In this section we focus on the 1D model where considerable progress in the understanding of the physical properties of the system can be gained by use of the powerful theoretical techniques of conformal field theory.[16] In particular, we will show how the exact solution for two and four particles, previously discussed, can be used

to evaluate analytically the correlation exponents in the zero-density limit. Then, we will evaluate the critical exponents for several choices of the parameters at quarter filling by a finite-size scaling analysis.

The behavior of the model at low density appears to be markedly different for U smaller or larger than its critical value U_c [Eq. (6)]. In the former case, the analysis of the two-particle problem shows that a spin gap is present in the excitation spectrum of the model, and thus we expect that the spin-spin correlations decay exponentially. On the other hand, the charge excitation spectrum is expected to remain gapless, as shown by the absence of four-particle bound states. In this case, the model should fall in the universality class of the Luther-Emery model[17] and its correlation exponents are expressed in terms of the unique parameter K_ρ.[18] This exponent can be related to the compressibility of the model using the Haldane-Schulz equation

$$L\frac{\partial^2 E}{\partial N^2} = \frac{\pi}{2}\frac{u_\rho}{K_\rho}\,, \tag{13}$$

where u_ρ is the charge velocity of the system, which is associated with the long-wavelength charge excitations: $E_k \sim u_\rho k$. In particular, the long-distance behavior of the charge correlations at $2k_F$ is $C_\rho(x) \sim \cos(2k_F x)/x^{K_\rho}$ while the s-wave superconductive correlations decay as $\Delta(x) \sim x^{-1/K_\rho}$. The Luther-Emery model is characterized by a central charge $c = 1$ which is related to the leading finite-size corrections of the ground-state energy:

$$\frac{E}{L} = e_\infty - c\,\frac{\pi\, u_\rho}{6L^2}. \tag{14}$$

In the other regime, for $U > U_c$ [Eq. (6)], the bound state is not present anymore and both the spin and charge excitations are gapless, at least away from half filling, where umklapp processes are absent. This can be also checked by going to the $U \to \infty$ limit where the bond-charge model maps into a standard t-J model with $J = 4(t-\gamma)^2/U$. The t-J model at small J is known to be a Luttinger liquid[2] whose correlation exponents are again parametrized by K_ρ [Eq. (13)]. In this case, all the correlation functions of the model are characterized by a power law behavior: Both the spin and charge correlations at $2k_F$ decay as x^{-1-K_ρ} while the charge correlations at $4k_F$ fall as x^{-4K_ρ}. Also the Luttinger liquid is characterized by a central charge $c = 1$, but, in this case, the presence of long-wavelength gapless spin excitations modifies Eq. (14) into

$$\frac{E}{L} = e_\infty - c\,\frac{\pi\,(u_\rho + u_\sigma)}{6L^2}, \tag{15}$$

where u_σ is the spin velocity.

This field theoretical formalism allows for the analytical evaluation of the correlation exponents of our model in the zero-density limit, where use can be made of the exact results obtained for few particles in a finite system. The key assumption, explicitly verified in the Hubbard model where Bethe ansatz solution is also available, is that the zero-density limit of the physical properties of the model is correctly reproduced by fixing the total number N of particles in the system at a given lattice size L and then taking the $L \to \infty$ limit. Following this procedure, the ground-state energy of two and four particles at $U < U_c$ can be written as

$$E = E_b\frac{N}{2} + \frac{\pi^2}{24}t_{\rm eff}\frac{N^3}{L^2} - \frac{\pi^2}{6}t_{\rm eff}\frac{N}{L^2} + O(L^{-3}); \tag{16}$$

here use has been made of Eqs. (7) and (12). The charge velocity can be obtained by the $1/L$ expansion of the energy of a pair at total momentum $P = 2\pi/L$, which, via Eq. (11), is

$$u_\rho = \pi\frac{N}{L}t_{\rm eff}. \tag{17}$$

Equations (13), (16), and (17) give the zero-density limit of the K_ρ exponent at all $U < U_c$ [Eq. (6)]: $K_\rho = 2$ independent of U coinciding with the negative U Hubbard model result. Also the central charge c of the system can be calculated by use of Eqs. (16), (17), and (14). The resulting value for c is $c = 1$, which provides a consistency test of the method used. Therefore we can conclude that the system is in the Luther-Emery regime with a spin gap and diverging superconductive susceptibility. Remarkably, the critical exponents associated with the charge degrees of freedom are identical with those of a hard core boson gas, as expected from the physical picture of a dilute dimer gas.

At $U > U_c$, the one- and two-particle solution is sufficient to give the exact scaling of the energy and charge velocity as $L \to \infty$:

$$E = -4t + \frac{\pi^2}{3}t\frac{N^3}{L^2} - \frac{\pi^2}{3}t\frac{N}{L^2} + O(L^{-3}), \tag{18}$$

$$u_\rho = 2\pi\frac{N}{L}t. \tag{19}$$

These expressions give $K_\rho = 1/2$ and central charge $c = 1$, showing that the system is in the Luttinger liquid regime with correlation exponents identical to those of the $U \to \infty$ repulsive Hubbard model.

To summarize, the bond-charge model is characterized by two different phases in the low-density limit: a Luttinger liquid regime for $U > U_c$ with both charge-density-wave and spin-density-wave long-range correlations at $2k_F$ and a Luther-Emery phase dominated by superconductive fluctuations present at $U < U_c$.

V. $D = 1$ AT FINITE DENSITY

In order to understand whether the transition found at U_c for low density persists also at finite density n, we can make use of the weak-coupling renormalization group method[17] which is known to give the correct scaling and the exact critical exponents to leading order in the interaction parameters U/t and γ/t. In this case we set $\beta = 0$ so that the resulting Hamiltonian is quartic in fermion operators. The model is first linearized around the two Fermi points, giving rise to a general, spin isotropic, *g-ology* model with coupling constants $g_1, \ldots, g_4$ functions of the two physical parameters U/t and γ/t. The

renormalization group equations are then integrated and the weak-coupling phase diagram is obtained.[19] The correct result can be also obtained by noticing that, linearizing both interactions around the Fermi points, we get an effective Hubbard model with coupling constant $U_{\rm eff} = U + 8\gamma\cos(\pi n/2)$. In the Hubbard model, the phase boundary between the Luttinger liquid and the Luther-Emery phase (with long-range superconductive correlations) is known to be at $U_{\rm eff} = 0$, leading to the weak-coupling result

$$U_c(n) = -8\gamma\cos(\pi n/2) + O(\gamma^2) \qquad (20)$$

and the correlation exponents can be read off the known Hubbard results[16]

$$K_\rho = 1 - \frac{U + 8\gamma\cos(\pi n/2)}{4\pi\, t\, \sin(\pi n/2)} + O(U^2, \gamma^2). \qquad (21)$$

In order to go beyond a perturbative determination of the phase diagram, we have analyzed the properties of the model at quarter filling where an accurate finite-size scaling can be done. We have studied in detail the case $\beta = \gamma^2/t$. A first qualitative hint on the existence of the transition comes from the analysis of the symmetries of the ground state when boundary conditions corresponding to "open shells" in the noninteracting regime are chosen. In this case, the interaction is responsible for the splitting of the singlet-triplet degeneracy of the free-fermion limit, and in fact two different symmetries are found, according to the choices of the parameters. If γ is negative and U is sufficiently small, the ground state is always a singlet belonging to the totally symmetric sector, as expected from the picture of a Bose condensate of s-wave Cooper pairs. Instead, by increasing U, a level crossing is observed and the ground state is a triplet, odd under reflections. This sort of "Hund rule" has been already observed in the repulsive Hubbard model for fillings corresponding to "open shell" conditions.[20] We can tentatively associate the occurrence of the transition to the choice of parameters corresponding to this level crossing. Lanczos diagonalizations have been performed for 1D lattices of 8, 12, and 16 sites with periodic (8 and 16) or antiperiodic (12) boundary conditions in order to achieve the "open shell" condition. The size scaling of the spin gap, i.e., the difference between the lowest spin singlet state and the lowest triplet state, is shown in Fig. 2 together with a parabolic extrapolation to the thermodynamic limit. The data strongly suggest that the gap remains finite in all the cases where the ground state is a singlet (solid symbols) while if the ground state is a triplet (open symbols) the gap is seen to scale to zero in the thermodynamic limit. Similar conclusions can be drawn by the inspection of the density and magnetic structure factors. Two typical examples are shown in Fig. 3 for 8 electrons in 16 sites with antiperiodic boundary conditions and $\gamma = -0.5t$. The $U = 0$ case is characterized by a smooth magnetic structure factor, while the density correlations have a cusp at wave vector $2k_F$. This suggests that the spin degrees of freedom are gapped while charges are gapless and their correlations behave as at the Luther-Emery fixed point. This has to

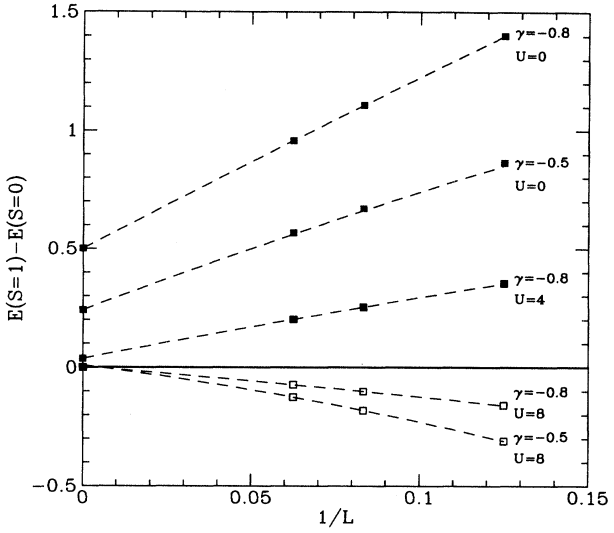

FIG. 2. Size scaling of the spin gap from Lanczos diagonalization in 1D at quarter filling. Boundary conditions correspond to open shells. Parameters are in units of t. Solid squares scale to a finite spin gap. Open squares scale to zero gap.

be contrasted with the behavior shown at $U = 8$ where also the spin structure factor shows a cusp at $2k_F$ while the singularity of charge correlations is considerably reduced. The shape of these correlation functions is quite similar to that of the Hubbard model[21] where both spin and charge degrees of freedom are gapless and the model scales to the Luttinger fixed point.

In order to be fully quantitative in the determination of the properties of the model, use can be made of the

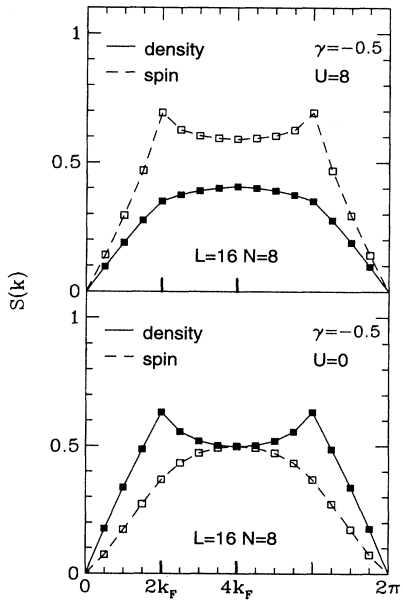

FIG. 3. Density and spin structure factors for two parameter choices in 1D at quarter filling.

TABLE I. Luttinger fixed-point exponents.

γ	U	K_ρ
0	4	0.71
0	8	0.62
−0.1	4	0.75
−0.1	8	0.64
−0.5	4	0.98
−0.5	8	0.78
−0.8	8	0.93

field theoretical expression (13) relating the correlation exponent K_ρ to easily computable quantities, like compressibility and charge velocity. The numerical evaluation of these quantities in a finite system can be straightforwardly obtained by

$$\frac{\partial^2 E}{\partial N^2} = \frac{E(N+2) - 2E(N) + E(N-2)}{4},$$
$$u_\rho = \frac{L}{2\pi}\left[E\left(P = \frac{2\pi}{L}\right) - E(P=0)\right]. \qquad (22)$$

Computations have been performed at quarter filling by use of "closed shell" boundary conditions (i.e., periodic for 12 sites and antiperiodic for 8 and 16 sites). In Figs. 4 and 5, we present the size scaling for the compressibility and the charge velocity for different values of U and γ obtained via Eq. (22) and a parabolic extrapolation to the thermodynamic limit. The resulting K_ρ is shown in Tables I and II where we have distinguished between parameters corresponding to a $K_\rho < 1$ (Luttinger liquid, Table I) and $K_\rho > 1$ (Luther-Emery, Table II). For $U = 0$ the system is always in the (quasi)superconducting region

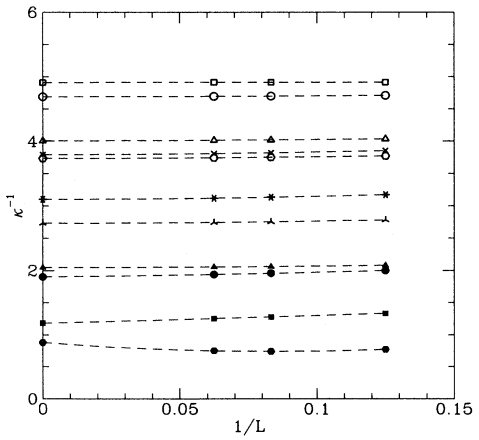

FIG. 4. Size scaling of the compressibility in $D = 1$ at quarter filling for different parameter choices of (γ, U) (in units of t): (0,4) (open triangles), (0,8) (open squares), (−0.1,0) (solid triangles), (−0.1,4) (open hexagons), (−0.1,8) (open circles), (−0.5,0) (solid squares), (−0.5,4) (skeletal triangles), (−0.5,8) (crosses), (−0.8,0) (solid hexagons), (−0.8,4) (solid circles), and (−0.8,8) (asterisks). The points at $L = \infty$ are obtained by a parabolic extrapolation of the Lanczos data.

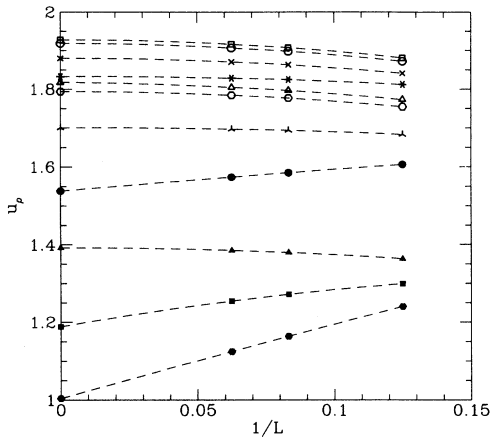

FIG. 5. Size scaling of the charge velocity. Symbols as in Fig. 4.

in agreement with the expectations, but superconductivity gets less and less robust for a density approaching half filling.

VI. MEAN-FIELD SOLUTION

The Hubbard model with correlated hopping was studied within BCS mean-field approximations in two and three dimensions by Hirsch and Marsiglio.[4–6] In order to compare mean-field theory with numerical diagonalization data, we briefly review the BCS equations for this model in arbitrary dimension for the choice $\beta = 0$ in Eq. (1). We also derive a closed expression for the critical value U_c^{BCS} which separates the superconducting ground state and the Luttinger (or Fermi) metal.

The interaction between Cooper pairs that arises from Hamiltonian (1) is given by the effective potential

$$V_{\mathbf{k}\mathbf{k}'} = U + 2\gamma \sum_\alpha (e^{i\mathbf{k}_\alpha} + e^{i\mathbf{k}'_\alpha}). \qquad (23)$$

For $\gamma < 0$, $V_{\mathbf{k}\mathbf{k}'}$ at the Fermi level becomes less and less negative as particles are added. So we expect that superconductivity in this model is favored at low density.

The BCS equations are

$$\Delta_{\mathbf{k}} = -\frac{1}{L^D}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}},$$
$$E_{\mathbf{k}} = \sqrt{(\tilde{\epsilon}_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2},$$
$$\tilde{\epsilon}_{\mathbf{k}} = -2t\left(1 - \frac{\gamma}{t}n\right)\sum_\alpha \cos(\mathbf{k}_\alpha),$$
$$n = 1 - \frac{1}{L^D}\sum_{\mathbf{k}} \frac{\tilde{\epsilon}_{\mathbf{k}} - \mu}{E_{\mathbf{k}}}. \qquad (24)$$

The form of the BCS equations implies that the gap $\Delta_{\mathbf{k}}$ depends on the wave vector $\mathbf{k}$ only through the free-particle dispersion $\epsilon_{\mathbf{k}}$ and this dependence is simply linear. Therefore $\Delta_{\mathbf{k}}$ can be parametrized by the two unknowns Δ and χ:

TABLE II. Luther-Emery fixed-point exponents.

γ	U	K_ρ
−0.1	0	1.07
−0.5	0	1.58
−0.8	0	1.78
−0.8	4	1.27

$$\Delta_{\mathbf{k}} = \Delta \left[1 + \chi \sum_{\alpha} \cos(\mathbf{k}_\alpha) \right] \tag{25}$$

and Eqs. (24) reduce to a set of coupled equations for Δ, χ, and the chemical potential μ which must be solved numerically. However, the critical line between the superconducting and the normal state can be obtained analytically by looking for a vanishing solution: $\Delta \to 0$. In the analysis of this limit of the BCS equations it is important to keep also the subleading term in $\chi \sim 2(t-\gamma n)/\mu + O(\frac{1}{\ln \Delta})$ in order to get the correct asymptotic result. In this way it is possible to obtain, for arbitrary dimension, a closed expression for the critical value:

$$U_c^{\mathrm{BCS}}(n) = \frac{4\gamma\mu}{t-\gamma n} + \frac{2\gamma^2}{(t-\gamma n)^2} \int \frac{d^D\mathbf{k}}{(2\pi)^D} |\tilde{\epsilon}_{\mathbf{k}} - \mu|, \tag{26}$$

which coincides with the exact low-density result (6) in the limit $n \to 0$. In fact, the BCS variational procedure becomes exact for two particles. Moreover, at weak coupling only the first term in (26) survives and the exact renormalization group result (20) is correctly reproduced. Notice that in the BCS approximation the critical U does not vanish at half filling but tends to a finite limit which, in 1D, is $U_c(n) = 8\gamma^2/\pi(t-\gamma)$. The model (1) and its mean-field phase boundary (26) are defined in arbitrary dimension D and have a smooth limit for $D \to \infty$ provided both the hopping and the bond-charge interaction are rescaled as $t \to t^*/(2D)^{1/2}$ and $\gamma \to \gamma^*/(2D)^{1/2}$.[22] Due to the simple form of the density of states in the $D \to \infty$ limit, Eq. (26) can be analytically evaluated as

$$U_c(n) = \frac{2\gamma^*\mu^*}{t^*}\left(2 - \frac{\gamma^*(1-n)}{(t^*-\gamma^* n)}\right) + \frac{4\gamma^{*2}}{(t^*-\gamma^* n)} \frac{e^{-(\mu^*/t)^2/2}}{\sqrt{2\pi}}, \tag{27}$$

where the chemical potential μ^* is related to the density by

$$n = 1 - \mathrm{erf}\left(\frac{-\mu^*}{t\sqrt{2}}\right). \tag{28}$$

In Fig. 6 we show how the BCS phase boundary is modified when the dimensionality D grows from 1, 2, 3 to ∞. In particular, we notice that the critical U at zero density increases as $\sqrt{D}$ and, at $D = \infty$, the critical line has a singularity at $n = 0$. As D increases, the superconducting region is pushed to lower densities but tends to a finite limit in the whole density axes up to $n = 1$.

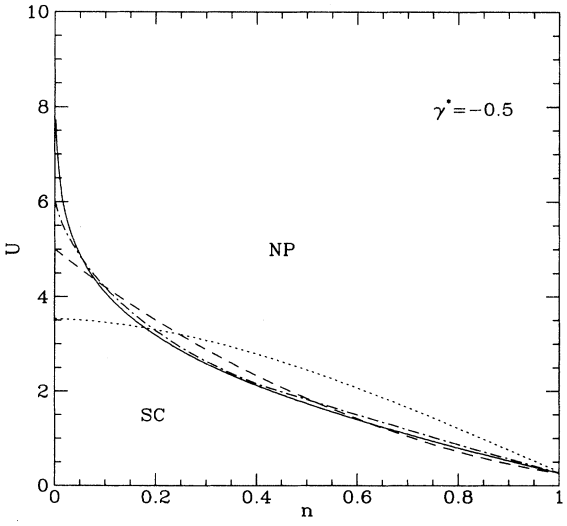

FIG. 6. Mean-field phase boundary between a superconducting (SC) and a normal (NP) phase in BCS approximation for $D = 1$ (dotted line), $D = 2$ (dashed line), $D = 3$ (dot-dashed line), and $D = \infty$ (solid line).

VII. PHASE DIAGRAM

In Fig. 7 we show the 1D zero-temperature phase diagram in the (U, n) plane resulting from the combination of the various techniques reported before, for $\beta = 0$ and

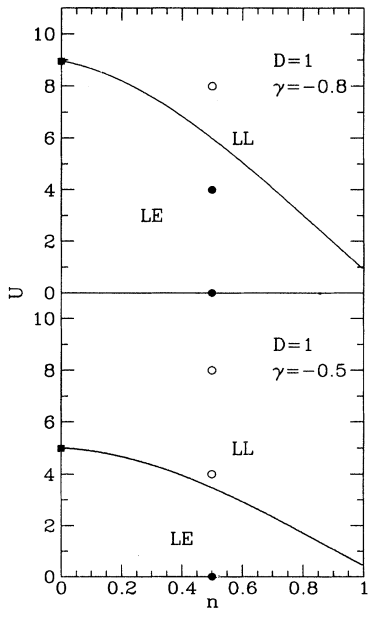

FIG. 7. 1D phase diagram of the model 1 at zero temperature, for $\beta = 0$ and two choices of $\gamma < 0$. The solid line is the BCS result separating a Luther-Emery (LE) region from a Luttinger liquid (LL) regime. The solid square is the exact zero-density limit. Circles are Lanczos results. Open symbols correspond to the Luttinger liquid, solid circles to the Luther-Emery phase.

two different values of parameter γ. The solid line shows the phase boundary in the mean-field approximation, as obtained in the previous section. Its zero-density limit is an exact result. Symbols represent numerical results at quarter filling obtained by finite-size scaling of Lanczos diagonalizations. In particular, solid circles correspond to the Luther-Emery phase while open circles represent the Luttinger liquid. The numerical data shown in these figures are quite consistent with the mean-field estimate of the critical line, giving us confidence in the BCS variational procedure for this class of systems.

The 2D model can be studied both within mean-field theory and by Lanczos diagonalizations. The critical line in the BCS approximation has been obtained in the previous section and is shown in Fig. 8 for $\beta = 0$ and two choices of γ. Again we remark that the zero-density limit is an exact result and coincides with what has been found via the two-particle analysis. Mean-field theory predicts a nonzero critical U_c also at half filling. The superconducting region, below the critical line, has a spin gap and true (off-diagonal) long-range order, while above the critical line the model is in a Fermi liquid regime. In order to test this mean-field phase diagram, we have carried out Lanczos diagonalizations also in the 2D model. In this case, however, a finite-size scaling of the results is not possible, due to the exceedingly large Hilbert space dimensions, and our analysis is limited to a 4×4 lattice. The results of the numerical analysis at quarter filling are shown in the same figure by solid circles if the system turns out to be in the superconducting region and by open circles if it is a Fermi liquid. The method we have used for extracting this information from the diagonalization data is quite similar to the one adopted in one dimension. The 4×4 lattice with 8 electrons, zero magnetization, and periodic boundary conditions is 16 times degenerate in the noninteracting case ($U = \gamma = 0$). However, interactions split this degeneracy, favoring some of the zero-momentum states: The positive U Hubbard model has a singlet ground state with d-wave symmetry[23] while a BCS superconducting state is expected to have s-wave symmetry. Therefore, a level crossing between these two (spatial) symmetries would suggest a change in the physical nature of the ground state, i.e., the crossing of the phase boundary between a Fermi liquid and a superconductor. Other, more conventional, methods for investigating the properties of the state, like the study of the spin gap or the analysis of the correlation functions, are strongly affected by the limitations in the lattice size and require a careful size scaling in order to give reliable results. Instead, the level crossing gives a clear-cut indication of a change in the structure of the ground state. For comparison, the correlation functions are shown in real space in Fig. 9 for a few parameter choices. This picture suggests the formation of structure in the spin distribution when U increases (i.e., when the model enters the Fermi liquid regime). The symmetry-based analysis leads us to the identification of the phases of the model for different choices of the parameters. The results, shown in Fig. 8, compare rather favorably with the BCS variational predictions, supporting the existence of a phase transition between a superconducting and a Fermi liquid phase in the 2D model at finite density. The character of the superconductive phase will probably change smoothly with increasing density, going from a dimer gas at low density to a regime of weakly bound Cooper pairs, similar to the usual BCS picture.

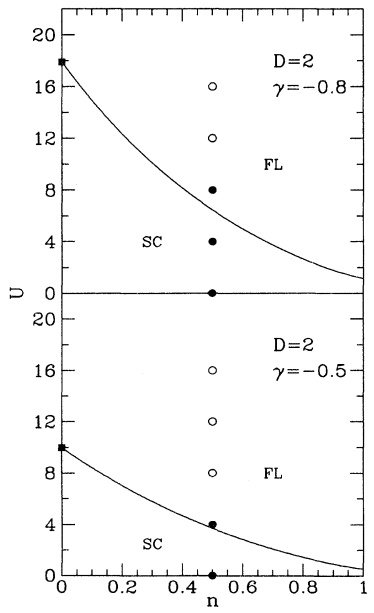

FIG. 8. 2D phase diagram. Notation as in Fig. 7. Here the two phases represent a superconductor (SC) and a Fermi liquid (FL).

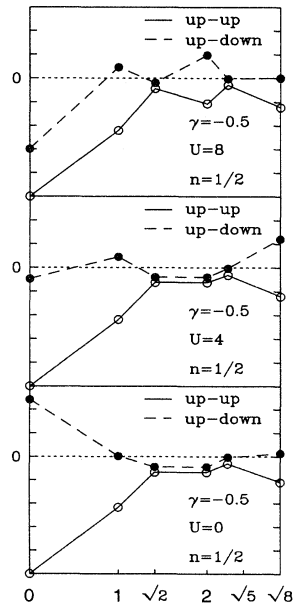

FIG. 9. Real space correlation functions in a 4×4 cluster at quarter filling. The uncorrelated part $\langle n_\sigma \rangle \langle n_{\sigma'} \rangle = 1/16$ has been subtracted.

In summary, we have studied a simple tight-binding model characterized by on-site Hubbard repulsion and nearest-neighbor bond-charge interaction. We have presented analytical and numerical results both in one and two dimensions, showing the presence of a phase transition at zero temperature between a superconducting region at small U and a Fermi liquid regime at larger repulsions. Superconductivity is rather insensitive to the Hubbard U due to the *off-diagonal* nature of the interaction responsible for binding. In 1D the analysis is much more rigorous due to the many powerful tools available, including weak-coupling renormalization group and conformal field theory. In the 1D case, no long-range order can be present in the model and the phase transition occurs between a Luther-Emery regime (quasisuperconducting) and a Luttinger liquid phase (quasi Fermi liquid). The correlation exponents and a quantitative characterization of the different phases are obtained by use of Lanczos diagonalizations combined with field theoretical techniques. A BCS variational analysis is in good agreement with the exact results presented in this work and reproduces the main features of the zero-temperature phase diagram. The analytical study of the few-particle problem leads to a physical picture of the superconductive phase in terms of a superfluid dimer gas both in one and two dimensions and, in 1D, allows for the quantitative evaluation of the correlation exponents.

After completion of this work, we received an unpublished report by Arrachea *et al.*[24] where the same model is numerically investigated in 1D and some of the results discussed in this paper are also obtained. In addition, here we provide (i) a detailed analysis of the low-density limit, (ii) an accurate finite-size scaling of the critical exponents in 1D, (iii) an analytic treatment of the phase diagram of the model at the mean-field level, (iv) the $D \to \infty$ limit, and (v) the numerical analysis in 2D.

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