One-dimensional pair hopping and attractive Hubbard models: A comparative study

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The low-energy physics of the one-dimensional pair hopping (PH) and attractive Hubbard models are expected to be similar. Based on numerical calculations on small chains, several authors have recently challenged this idea and predicted the existence of a phase transition at half filling and finite positive coupling for the pair-hopping model. We reexamine the controversy by making systematic comparisons between numerical results obtained for the PH and attractive Hubbard models. To do so, we have calculated the Luttinger parameters (spin and charge velocities, stiffnesses, etc.) of the two models using both the density matrix renormalization-group method for large systems and Lanczós calculations with twisted boundary conditions for smaller systems. Although most of our results confirm that both models are very similar we have found some important differences in the spin properties for the small sizes considered by previous numerical studies (6–12 sites). However, we show that these differences disappear at larger sizes (14–42 sites) when sufficiently accurate eigenstates are considered. Accordingly, our results strongly suggest that the ground-state phase transition previously found for small systems is a finite size artifact. Interpreting our results within the framework of the Luttinger liquid theory, we discuss the origin of the apparent contradiction between the predictions of the perturbative renormalization-group approach and numerical calculations at small sizes. [S0163-1829(96)05047-3]

I. INTRODUCTION

In this paper we are concerned with the pair-hopping (PH) model described by the Hamiltonian

$$H=-t\sum_{\langle i,j\rangle\sigma}[c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c}]-V\sum_{\langle i,j\rangle}[c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}c_{j\downarrow}c_{j\uparrow}+\text{H.c.}], \tag{1.1}$$

where $c_{i\sigma}^{\dagger}$ ($c_{i,\sigma}$) creates (destroys) a fermion of spin σ ($\sigma=\uparrow,\downarrow$) at lattice site i. The first term is the usual kinetic energy term (tight-binding approximation), the V term allows spin-singlet pairs of electrons to hop from site to site. In what follows, we shall restrict our study to the case $V>0$.[1]

There are a number of reasons that make this model interesting to study. First, the pair-hopping model can be viewed as a phenomenological model to describe the dynamics of small size Cooper pairs. Since high-T_c superconductors are known to display such pairs, to study this model can be important to capture some of the physics of these materials. Of course, when working with such a model nothing is said about the nature of the underlying mechanism responsible for the tight binding of the pairs. Second, it can be shown that the pair-hopping term arises from Coulomb interaction at large negative U in the Hubbard model.[2,3] Accordingly, the competition between the usual one-electron hopping and pair hopping is related to the physics of the Hubbard model at strong coupling. Finally, understanding the physics resulting from all possible unusual interactions in one-dimensional (1D) strongly correlated models is clearly a problem of central importance in solid-state physics.

Very recently this model has led to some contradictory results. Using exact diagonalization calculations on small 1D chains (up to $L=10$ sites, with periodic boundary conditions), Penson and Kolb claimed[4] that a phase transition should occur at some finite critical value of the hopping parameter V with $V_c/t\sim 1.4$. More precisely, they showed that a gap in the single-particle spectrum of the half-filled system opens up at that value. They have also observed that the second derivative of the ground-state energy with respect to V (a quantity similar to a specific heat) has a local maximum at the transition, which seems not to diverge. This would indicate a phase transition with an essential singularity. Very soon after, Affleck and Marston,[5] making a renormalization-group analysis with bosonization methods of the PH model, showed that, in the continuum limit (low-energy, long-distance physics), this model is essentially equivalent, up to some irrelevant terms, to the negative-U Hubbard model, the only important difference lying in the bare coupling constants. Accordingly, they predicted that the transition in the pair-hopping model must occur at $V=0$ just as in the Hubbard model, the finite value observed in the numerical calculations for very small chains being attributed to a finite-size artifact. A few years later, Hui and Doniach[6] presented some numerical calculations analyzed with more sensitive tools than the standard finite-size scaling analysis based on very small samples. Using an eigenprojection decomposition of the different order parameter operators involved and also some calculations of the helicity modulus, they found that the data seemed indeed to be compatible with the existence of a phase transition at a finite value of V, thus in contradiction with the weak-coupling renormalization-group results. They also presented some arguments as to why the predic-

tions of the renormalization-group analysis of Affleck and Marston could be not valid. Very recently, Bhattacharyya and Roy[7] have investigated the PH model using a real-space renormalization-group method. At small positive V they also found the existence of a gapless phase (identified as a quasimetallic phase dominated by short-range superconducting correlations), which disappears at some finite value of the coupling. Finally, Sikkema and Affleck[8] have presented some numerical results for the one-particle gap as a function of V using the density matrix renormalization-group (DMRG) method with open boundary conditions. Using samples up to $L=60$, they concluded that there is no spin-gap transition at a nonzero positive value of V and that the standard low-energy picture given by the perturbative renormalization-group approach is valid. Although we reach in this work essentially the same conclusions, we shall follow here a quite different route. In particular, our DMRG calculations are done with periodic boundary conditions (PBC) instead of open BC. This will allow us to study in detail the very peculiar behavior of the pair hopping at small couplings (large correlation lengths). This point is discussed in Sec. IV.

At the heart of the controversy is the question of knowing whether the long-distance, low-energy physics of the pair-hopping model is different from that of the usual attractive Hubbard model. As we shall see in the next section all standard approaches lead to the same conclusion: the low-energy sector of both Hamiltonians should be similar under the trivial correspondence $U=-2V$. At half filling it is known (an exact result) that no phase transition at a nonzero value of U exists for the attractive Hubbard model. How can the PH model exhibit a different behavior? This should result from a highly nontrivial process involving nontrivial excitations. Note also that the exotic gapless phase is supposed to exist at an arbitrary small value of the hopping parameter, a domain where the high-energy degrees of freedom are not expected to play an important role. In order to settle down the controversy we propose to make a systematic comparison of the physics of the pair-hopping and attractive Hubbard models at low energy. To do so, we have calculated the spin and charge velocities of the two models using both the density matrix renormalization-group method with periodic boundary conditions for large systems and Lanczós calculations with twisted boundary conditions for smaller systems. Our results show that there are some important differences in the finite-size behavior of the two models. Using the framework of the Luttinger liquid we propose an interpretation of the origin of the controversy between the perturbative RG prediction and the numerical results for small chains presented up to now.

The paper is structured in the following way. In Sec. II, we briefly present the results of a number of approaches illustrating the very close similarity between the attractive Hubbard model and the pair-hopping model. In Sec. III, we present our numerical results using the Luttinger liquid theory and the twisted boundary conditions method on both models for chains up to $L=12$ sites. Then, using the DMRG method we generalize the results presented for small chains at some larger chains up to $L=42$ sites. In Sec. V, we discuss the results and comment on what we believe to be the origin of the controversy. We conclude that (1) both models are indeed equivalent at low energy in the thermodynamic limit and that there is no phase transition at finite V and half filling in the PH model and (2) for small systems there exists a transient regime specific to the PH model and responsible for the unconventional behavior of this model.

II. PAIR-HOPPING AND ATTRACTIVE HUBBARD MODELS

The Hamiltonian (1.1) for the pair-hopping model describes a competition between the usual kinetic term (t term) corresponding to single-electron hopping and a V term corresponding to the hopping of spin-singlet pairs, the range of both types of hopping being limited to nearest neighbors. When V/t is large ($V>0$), the pair-hopping term dominates and the model becomes equivalent to spinless fermions (for an even number of electrons). The ground state is massively paired and there is a gap of order V in the one-particle spectrum (binding energy of the pairs). In the opposite limit, $V/t \ll 1$, the one-particle hopping dominates and the pairs tend to be destroyed. This type of competition is very similar to that encountered in the attractive Hubbard model described by the Hamiltonian

$$H=-t\sum_{\langle i,j\rangle\sigma}[c^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.}]+U\sum_{i} n_{i\uparrow}n_{i\downarrow}. \tag{2.1}$$

Here also we have a competition between a one-electron hopping and the formation of spin-singlet pairs. However, in contrast with the PH model, pairs have no intrinsic mobility (uncorrelated mobility via the t term). The physics of the attractive Hubbard model is well understood since this model admits an exact solution via the Bethe ansatz technique. In particular, it is known that the effect of the on-site interaction is rather drastic: a gap in the one-particle spectrum opens up for any nonzero value of the interaction U (negative or positive) at half filling. It is usually thought that a similar situation should occur in the PH model. This opinion is supported by the fact that standard approximate approaches applied to both Hamiltonians lead quite systematically to the same physics at low energy under the trivial correspondence $U\leftrightarrow -2V$. However, as already emphasized, this idea has been recently challenged. The purpose of the next few sections is to shed some light on this controversy. Here, we would like to briefly illustrate, by applying some standard methods, why the correspondence between both models is usually taken for granted.

A first approach to consider is the mean-field approximation. Defining the superconducting order parameter by $\Pi=\langle gnd|c_{i\downarrow}c_{i\uparrow}|gnd\rangle$, where $|gnd\rangle$ denotes the BCS-type ground state, we consider the quantum fluctuations around this value and construct the approximate mean-field Hamiltonian by keeping only the terms that are of first order with respect to the fluctuations. The following Hamiltonian is obtained:

$$H_{\text{MF}}=\sum_{\mathbf{k},\sigma}\varepsilon(\mathbf{k})c^{\dagger}_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}-4V\Pi D\sum_{\mathbf{k}}[c^{\dagger}_{\mathbf{k},\uparrow}c^{\dagger}_{-\mathbf{k},\downarrow}+c_{\mathbf{k},\downarrow}c_{-\mathbf{k},\uparrow}]+4V\Pi^2 DL^D, \tag{2.2}$$

where $\varepsilon(\mathbf{k})=-4t\Sigma_{\mu=1}^{D}\cos(\mathbf{k}\cdot\mathbf{e}_{\mu})$, $\mathbf{e}_{\mu}$ being the unit vector in direction μ, and D the dimension of space. The main observation is that this Hamiltonian is identical to that obtained in the case of the Hubbard model[9] with the substitu-

tion $U=-2V$. Introducing the elementary excitations in the usual way, we can compute the dependence of the gap Δ in energy of the system, we get

$$\Delta \sim te^{-ct/|V|} \quad \text{for } V\to 0, \text{ where } c \text{ is a positive constant}$$

and

$$\Delta \sim V \quad \text{for } V\to\infty. \tag{2.3}$$

Clearly, in this approach both models are equivalent and the gap opens up at $V/t=0$ with a standard behavior.

We have also considered the large-dimension limit of the pair-hopping model. This recent approach can be seen as a sort of dynamical mean-field theory. Although this limit may seem rather academic, practical calculations have illustrated the fact that a great part of the physics of low-dimensional systems is captured.[10,11] Once again, in that approximation we have found that the equations reduce to those of the corresponding attractive Hubbard model with $U=-2V$. In fact, this is not really surprising since, because of the structure of the Fermi hypersurface in the limit of large dimensions, the effects of the high-energy excitations that could be responsible for nontrivial processes are strongly suppressed.

As we shall see in Sec. V the renormalization-group (RG) flows in the weak-coupling limit are also identical for the two models [Eq. (5.1)] with, here also, the same correspondence between couplings. Only the initial values of the coupling constants, are model dependent.

Finally, one can try to find out whether the PH model has an exact solution via the Bethe ansatz. The essential step is to compute the two-particle S matrix from the Schrödinger equation and then to verify whether the S matrix satisfies the Yang-Baxter condition. Denoting by $A_{\sigma_1,\sigma_2}(p_1,p_2)$ the amplitude of the two-particle wave function written in terms of a combination of plane waves, defining as usual the two-particle S matrix as

$$A_{\sigma_2,\sigma_1}(p_2,p_1)=\sum_{\sigma_1',\sigma_2'} S^{\sigma_1,\sigma_1'}_{\sigma_2,\sigma_2'}(p_1,p_2)A_{\sigma_1',\sigma_2'}(p_1,p_2), \tag{2.4}$$

forcing the wave function to obey the Schrödinger equation, and imposing the continuity condition of the wave function, we get the following expression for the S matrix:

$$\begin{aligned} S^{\sigma_1,\sigma_1'}_{\sigma_2,\sigma_2'}(p_1,p_2)=&\frac{\sin ap_1-\sin ap_2}{\sin ap_1-\sin ap_2-iV\cos[a(p_1+p_2)]}\\ &\times\delta_{\sigma_1,\sigma_1'}\delta_{\sigma_2,\sigma_2'}\\ &-\frac{iV\cos[a(p_1+p_2)]}{\sin ap_1-\sin ap_2-iV\cos[a(p_1+p_2)]}\\ &\times\delta_{\sigma_1,\sigma_2'}\delta_{\sigma_2,\sigma_1'}. \end{aligned} \tag{2.5}$$

It is easy to verify that the S matrix just given does not satisfy the Yang-Baxter condition.[12] Now, the important point is that the S matrix (2.5) is identical to that of the Hubbard model with the substitution $U\to -2V\cos[a(p_1+p_2)]$. The lattice spacing a gives a natural high-energy cutoff, $1/a$, in the problem. In the low-energy regime, i.e., $p_i \ll 1/a$, both approaches lead to the same equations and the two models related by $U=-2V$ should be equivalent.

To summarize, mean-field approximation, large-D limit, weak-coupling renormalization-group, and Bethe ansatz approaches indicate that the PH model and the $U=-2V$ attractive Hubbard model should be equivalent in the low-energy regime.

III. LUTTINGER LIQUID BEHAVIOR: AN EXACT DIAGONALIZATION STUDY ON SMALL SYSTEMS

In this part we are interested in evaluating the Luttinger liquid parameters for both the pair-hopping and attractive Hubbard models. As is well known the long distance behavior of one-dimensional gapless fermion systems can be studied by making use of the concept of ''Luttinger liquid.'' Within the framework of this theory the low-energy properties are given by an effective Luttinger model describing collective spin and charge density oscillations. The general form of the effective Hamiltonian can be obtained by writing the 1D fermion model in momentum space, restricting excitations and interactions to lie close to the Fermi surface, and looking for the important processes. As is well known only four processes survive (in the renormalization-group sense): one describing backward scattering of oppositely moving electrons with coupling g_1, one describing forward scattering of oppositely moving electrons with coupling g_2, one describing umklapp scattering with coupling g_3, and, finally, one describing forward scattering of electrons moving in the same direction with coupling g_4. (Notations are those of Refs. 13 and 14.) Taking the continuum limit of the fermion Hamiltonian and, then, bosonizing the Fermi fields, one gets

$$H_b=H_\rho+H_\sigma+H_1+H_3, \tag{3.1}$$

where H_ν ($\nu=\rho,\sigma$) are two free Bose Hamiltonians describing the spin ($\nu=\sigma$) and charge ($\nu=\rho$) collective excitations:

$$H_\nu=\int dX\left[\frac{u_\nu}{2\pi K_\nu}(\partial_X\phi_\nu)^2+\frac{u_\nu\pi K_\nu}{2}\Pi_\nu^2\right] \tag{3.2}$$

and H_1 and H_3 are the terms corresponding to the backward and umklapp scattering contributions, respectively,

$$H_1=\frac{2g_1}{(2\pi\alpha)^2}\int dX\cos(\sqrt{8}\phi_\sigma) \tag{3.3}$$

and

$$H_3=\frac{2g_3}{(2\pi\alpha)^2}\int dX\cos(\sqrt{8}\phi_\rho). \tag{3.4}$$

Here, ϕ_ρ (ϕ_σ) is the Bose field describing the charge (spin) excitations, and Π_ρ (Π_σ) is its canonical conjugated field. The coefficients u_ρ (u_σ) are the charge (spin) excitation velocities, and the parameters K_ρ and K_σ are some constants that can be shown to be related to the (nonuniversal) exponents of the power-law behavior of the correlation functions. In Eqs. (3.3) and (3.4) α is a short-distance cutoff.[14]

In the free-fermion case, $K_\rho=K_\sigma=1$ and $u_\rho=u_\sigma=v_F=2t\sin[(\pi/2)n]$, where $n=N/L$ is the electron density. When interactions are switched on, the u and the K param-

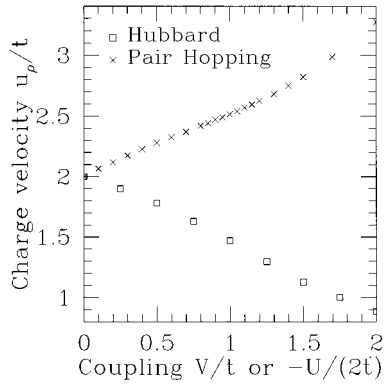

FIG. 1. Charge velocity u_ρ as a function of the coupling. Crosses, pair-hopping model, squares, Hubbard model. Lanczós calculations with twisted boundary conditions. Chains of sizes up to 12 sites.

eters are renormalized. In particular, the two velocities become different, charge and spin excitations do not propagate at the same speed. This phenomenon is known as the spin-charge separation in one-dimensional systems. All the details concerning the Luttinger liquid theory can be found, e.g., in Refs. 14 and 13 and references therein.

In order to compute numerically the Luttinger coefficients, we have used their expressions in terms of spin and charge compressibilities and stiffnesses of the system. More precisely, for the charge degrees of freedom we have

$$\frac{1}{\kappa}=\frac{\pi}{2}\frac{u_\rho}{K_\rho},\quad D_\rho=2u_\rho K_\rho, \tag{3.5}$$

where κ is the compressibility of the system and D_ρ is the charge stiffness, and for the spin degrees:

$$\frac{1}{\chi}=\frac{\pi}{2}\frac{u_\sigma}{K_\sigma},\quad D_\sigma=2u_\sigma K_\sigma, \tag{3.6}$$

where χ is the spin susceptibility of the system and D_σ the spin stiffness. These quantities can be computed from the spectrum of the system by using the relation[15]

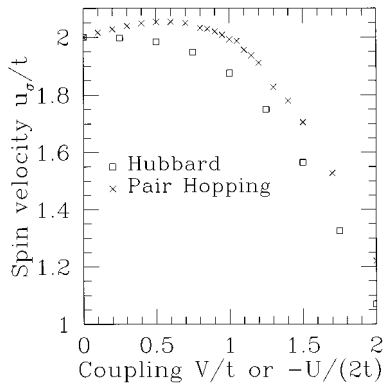

FIG. 2. Spin velocity u_σ as a function of the coupling. Crosses, pair-hopping model; squares, Hubbard model. Lanczós calculations with twisted boundary conditions. Chains of sizes up to 12 sites.

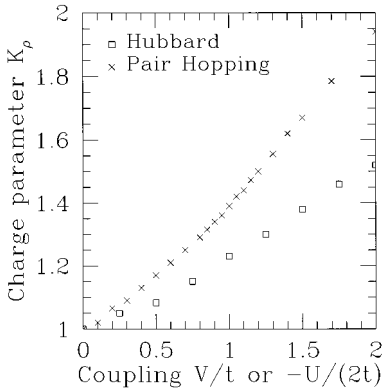

FIG. 3. Charge parameter K_ρ as a function of the coupling. Crosses, pair-hopping model; squares, Hubbard model. Lanczós calculations with twisted boundary conditions. Chains of sizes up to 12 sites.

$$D_\nu=\pi\left.\frac{\partial^2 E_0}{\partial\varphi_\nu^2}\right|_{\varphi_\nu=0}, \tag{3.7}$$

where φ_ρ is a charge twist in the system [i.e., the system has twisted boundary conditions such as $c^\dagger_{j+L,\sigma}=\exp(i\varphi_\rho)c^\dagger_{j,\sigma}$], and φ_σ is a spin twist in the system [i.e., $c^\dagger_{j+L,\sigma}=\exp(i\sigma\varphi_\sigma)c^\dagger_{j,\sigma}$], and

$$\frac{1}{\kappa}=\frac{1}{2L}\frac{\partial^2 E_0}{\partial n^2},\quad \frac{1}{\chi}=\frac{1}{2L}\frac{\partial^2 E_0}{\partial s_Z^2}, \tag{3.8}$$

with $n=(N_\uparrow+N_\downarrow)/L$ and $s_Z=(N_\uparrow-N_\downarrow)/L$. By computing these quantities for different values of the interaction, we can deduce the behavior of the Luttinger parameters u_ν and K_ν as a function of the coupling strength.

We have applied this approach to systems of sizes ranging from $L=4$ to $L=12$. The ground-state energies have been calculated using a standard Lanczós procedure. The results are presented in Figs. 1–5. Each figure shows the variation of the corresponding Luttinger coefficient as a function of the interaction, both for the attractive Hubbard model (squares) and for the pair-hopping model (crosses). Figure 1 gives the variation of the charge velocity, u_ρ, as a function of U or V. At small coupling both curves are linear with a

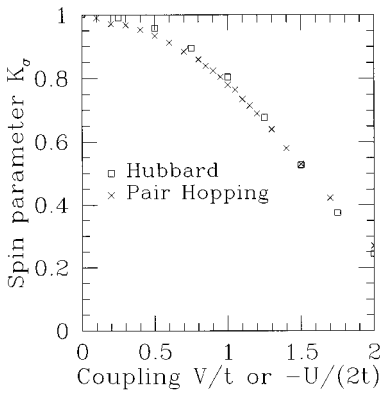

FIG. 4. Spin exponent K_σ as a function of the coupling. Crosses, pair-hopping model; squares, Hubbard model. Lanczós calculations with twisted boundary conditions. Chains of sizes up to 12 sites.

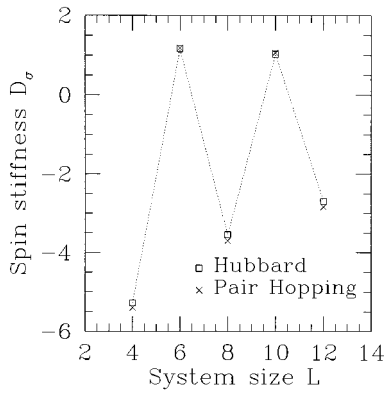

FIG. 5. Spin stiffness D_σ as a function of the coupling. Crosses, pair-hopping model, squares, Hubbard model. Lanczós calculations with twisted boundary conditions. Chains of sizes up to 12 sites. The dotted line is just a guide to the eye.

very good accuracy. More precisely, we find $u_\rho \sim 2+V/2$ and $u_\rho \sim 2+U/4$, for the pair-hopping and Hubbard models, respectively. For stronger couplings, small corrections to linearity show up. Both behaviors are typical of a regime with no charge gap. As we shall see later, these results are in perfect quantitative agreement with the prediction of the Luttinger liquid theory [Eqs. (5.2) and (5.3)]. Data for the spin velocities are rather different. As can be seen in Fig. 2 two distinct behaviors for the spin velocity are obtained. In the case of the attractive Hubbard model u_σ decreases uniformly from the free fermion value to zero at large coupling. In contrast, a maximum around $V=0.55t$ is found for the pair-hopping model. Both models recover a similar behavior between approximately $V=1$ and $V=1.5$. Note that the transition value observed in Refs. 4 and 6 lies within this interval. We shall discuss further this important difference of behavior for u_σ in Sec. V. Figures 3 and 4 demonstrate that the constants K_ρ and K_σ behave essentially the same way in both models. As already mentioned, in the Luttinger liquid theory these constants are related to the exponents of the power-law behavior of correlation functions. Accordingly, this common behavior would suggest that both models have the same phases. In Fig. 5, the behavior of the spin stiffness of the pair-hopping model as a function of the size is displayed. A very interesting feature is that this quantity can be exactly computed for the Hubbard model. The formula is[16]

$$D_\sigma(L)=(-1)^{L/2+1}L^{1/2}D(U)e^{-L/\xi_\sigma(U)}$$

with

$$\xi_\sigma^{-1}(U)=\frac{4}{U}\int_1^\infty dy\,\frac{\ln(y+\sqrt{y^2-1})}{\cosh(2\pi y/U)}$$

and

$$D(U)\sim\begin{cases}\sqrt{(2/\pi\xi_\sigma)} & \text{for } U\to 0\\ 0.147\,376U & \text{for } U\to\infty\end{cases} \tag{3.9}$$

This function is plotted in Fig. 5, for $U/t=-2$, with the corresponding quantity for the pair-hopping model, at $V/t=1$. The similarity between the two curves is striking. In the case of the Hubbard model, the oscillations around zero are related to the existence of a gap in the spin spectrum. In the case of a gapless mode, the corresponding curve is smooth and never changes sign. Accordingly, we have here strong evidence in favor of the existence of a spin gap in the pair-hopping model.

At this point, our results are contradictory. On one hand, most of the results indicate that both models are quite similar (behavior of u_ρ, K_ν, and spin stiffnesses). On the other hand, the spin velocities at small sizes for both models display a different behavior. A closer look at spin degrees of freedom at larger sizes is therefore necessary.

IV. LUTTINGER LIQUID BEHAVIOR: A DMRG STUDY FOR LARGER SYSTEMS

Conformal field theory (CFT) is a powerful theory to describe the physics of 1D quantum (or 2D statistical) critical systems. Once conformal invariance is supposed, CFT provides a general framework relating finite-size scaling of physical quantities to thermodynamic properties.[17–19] In this work we shall essentially compare our data for excitation gaps with the predictions of CFT. This will allow us to check whether or not our data are compatible with the existence of a critical regime for the pair-hopping model. Denoting ν the gapless excitation under consideration and u_ν the velocity of the corresponding critical mode, the finite-size scaling expression of the excitation gap Δ_ν predicted by CFT is

$$\Delta_\nu=\frac{2\pi u_\nu}{L}, \tag{4.1}$$

where L is the system size. For a finite system at a given filling, the spin gap is defined as

$$\Delta_\sigma=E_0(N_\uparrow+1,N_\downarrow-1)-E_0(N_\uparrow,N_\downarrow),$$

where N_σ is the number of σ-spin electrons. Physically, it gives the change in ground-state energy produced when flipping one spin, the charge number being kept fixed.

In order to calculate the spin gaps we have used the density matrix renormalization-group method.[20] DMRG is a powerful technique to compute low-energy properties of quantum lattice systems. This method has been applied with success to several problems including the spin-1/2 Heisenberg chains,[20] the spin-1 chains,[21] the one-dimensional Kondo insulator,[22] the two-chain Hubbard model,[23] etc. The results obtained are very accurate and the method allows one to treat systems of sizes a few times larger than those accessible with exact diagonalization techniques. Essentially, DMRG is a real-space numerical renormalization-group procedure. It differs from standard approaches in the way that states of individual blocks are chosen. Instead of keeping the lowest eigenstates of the block considered as isolated from the outside world, the kept states are the most probable eigenstates of the density matrix associated with the block considered as a part of the whole system. It is easy to show that doing this is equivalent to constructing the most accurate representation of the complete state of the system: block plus the rest of the system. For a detailed and very clear presentation of the method the reader is referred to Ref. 20. There exist different ways of choosing the configuration of blocks used for the density matrix calculations. In particular, this

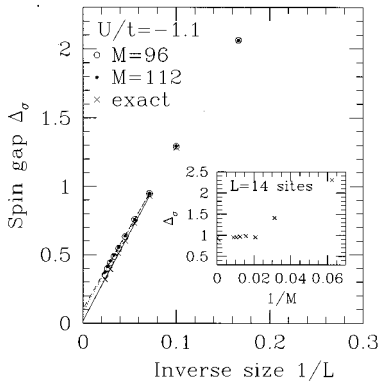

FIG. 6. Spin gap vs inverse of the system size for the attractive Hubbard model at $U/t=-1.1$ using DMRG with periodic boundary conditions for different values of M (see text). Inset shows the convergence of the spin gap as a function of M at $L=14$ sites. The value at $1/M=0$ is the exact value calculated by solving the Lieb-Wu equations.

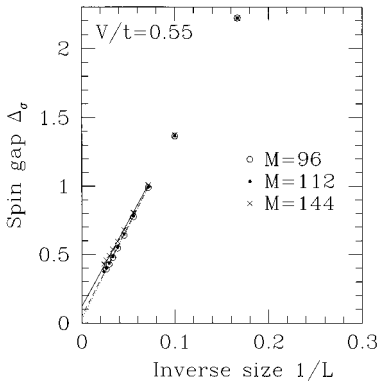

FIG. 7. Spin gap vs inverse of the system size for the pair-hopping model at $V/t=0.55$ using DMRG with periodic boundary conditions for different values of M (see text).

choice will depend on the type of boundary conditions used. Here, all calculations have been done by using periodic boundary conditions (PBC). We have chosen the superblock configuration $B_l \bullet B_l^R \bullet$ with $B'_{l+1}=B_l \bullet$ as proposed in Ref. 20 for PBC. B_l represents a block consisting of l sites, B_l^R is the reflected block (right interchanged with left), and $\bullet$ represents a single site. All notations are those of Ref. 20. In what follows we shall denote by M the number of eigenstates of the density matrix that are kept.

Very recently, Sikkema and Affleck have presented DMRG calculations for the pair-hopping model.[8] Their calculations have been performed using open boundary conditions (OBC). When the correlation length is finite and calculations with $L \gg \xi$ are possible using OBC is usually preferable (calculations with OBC are less demanding that with PBC, the convergence as a function of M being much more rapid). In the regime of small ξ, Sikkema and Affleck have shown that their data are consistent with the prediction of the standard perturbative RG flow. In this work we shall use PBC in a regime where the correlation lengths are large (small values of V). As we shall see now, this will allow us to study the very peculiar behavior of the pair-hopping model at small couplings.

To begin with we present some DMRG calculations for the attractive Hubbard model. The value of the Coulomb interaction, $U=-1.1$, has been chosen to correspond to $V=-U/2=0.55$, the value for which the spin velocity of the PH model is maximum; see Fig. 2. Since the Hubbard model admits an exact solution our results can be compared to the exact values obtained by solving the Lieb-Wu equations.[24] The inset of Fig. 6 shows how the DMRG spin gap Δ_σ converges to the exact value $\Delta_\sigma=0.9297$ for a chain of 14 sites as a function of M, the number of states kept. Here, M ranges from $M=16$ to $M=112$. Clearly, the convergence of the DMRG values is quite good. In addition, this curve provides a useful check of the validity of our code. The main plot displays the variation of the spin gap as a function of $1/L$. The studied sizes are ranging from $L=6$ to $L=42$. We did not consider the system sizes corresponding to a multiple of 4 since, in this case, the ground state is degenerate, thus causing a strong boundary frustration effect (which, of course, disappears in the $L\to\infty$ limit). For each size, we plot the value of the DMRG spin gap for a number of kept states $M=96$, $M=112$, and $M=\infty$ (exact Lieb-Wu value). Let us first consider the exact solution. Looking at the $L\to\infty$ limit, we observed a very small gap as expected. In this regime the systems considered ($L=6$–42) are in an effective quasicritical regime with a spectrum structure remaining close to the conformal tower structure. This allows us to write the following ansatz:

$$\Delta_\sigma(L)=\Delta_\sigma^\infty+\frac{2\pi u_\sigma}{L}, \tag{4.2}$$

valid in the regime $a \ll L \ll \xi$, and where u_σ should be considered as an effective spin velocity. The results obtained are in excellent agreement with the behavior predicted by formula (4.2) with a spin velocity very close to the free value. In addition, for small systems ($L=6,10$) the spin velocity obtained from the slope of the spin gap is in very good agreement with the value obtained in the preceding section (within 1.5%) based on a completely independent evaluation.

Let us now consider the DMRG results. We have observed that, for large enough values of M, the linear behavior of the spin gap as a function of $1/L$ is recovered. In Fig. 6 we show typical results for $M=96$ and $M=112$. The value of the spin velocity obtained from different M are displayed in Fig. 8 and are slightly smaller than the free value of 2. These results are consistent with a convergence to the exact value at large M. However, it is not possible from DMRG results to get an accurate estimate of the value of the gap itself. Indeed, although we have a good convergence of the results for a given size as a function of M (see inset of Fig. 6), the extrapolated value of the gap using different sizes is a very sensitive quantity. In fact, it is not reasonable to discriminate between a small but finite gap and a strictly vanishing gap. We clearly see in Fig. 6 that the extrapolated gap is not at all converged as a function of M. In order to get converged values we would need much larger values of M, which are clearly beyond of reach of present computers.

In Fig. 7 we present DMRG calculations for the pair-hopping model at $V=0.55$. Results of the spin gap as a func-

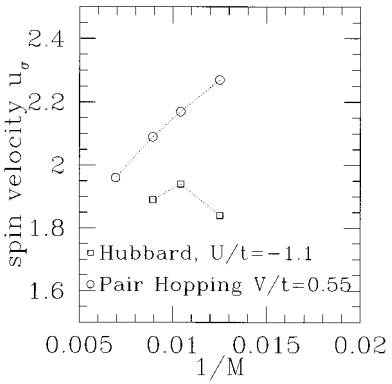

FIG. 8. Spin velocity u_σ computed from DMRG data as a function of $1/M$.

tion of $1/L$ are presented for $M=96$, 112, and 144. Here again we clearly see a quasicritical regime very well described by formula (4.2). As already emphasized for the attractive Hubbard model, the accessible values of M do not allow a direct conclusion on the existence or not of a finite spin gap. However, the data provide an estimate of the effective spin velocity via the slope of the curves. The spin velocities obtained are plotted for $M=84$, 96, 112, and 144 in Fig. 8. It is remarkable that the results are rather different for both models. As already noticed, for the Hubbard model the values of u_σ are slowly varying and always smaller than the free fermion value. In contrast, for the PH model u_σ is quite important for small values of M and decreases uniformly for increasing M. Only when large enough values of M are used, spin velocities of both models become comparable. We shall comment more on this point in the next section.

V. DISCUSSION

Let us summarize the results obtained. For small sizes ($L=4-12$) we have computed the Luttinger parameters $u_\rho, u_\sigma, K_\rho, K_\sigma, D_\rho$, and D_σ as a function of the interaction for both the attractive Hubbard and pair-hopping models. Regarding charge degrees of freedom all results for both models are consistent with the existence of a vanishing charge gap for arbitrary values of the interaction and with the fact that the low-energy charge sectors of both models are very similar. These results are in agreement with the conclusions of previous works.

Now, regarding spin degrees of freedom the situation is not so clear. For small sizes our results show that parameters K_σ and D_σ for both models are almost identical (see Figs. 4 and 5). In particular, in the case of the PH model we clearly see the oscillations of D_σ around zero as a function of the size L, a behavior that is usually interpreted as resulting from the existence of a gap. However, data for the spin velocity of the PH model do not display the expected behavior of a system with a gap. In contrast with the case of the attractive Hubbard model for which u_σ decreases uniformly from the free fermion value to zero at large coupling (a typical behavior for a finite system with a finite gap in the thermodynamic limit), we have observed a clear enhancement of u_σ when the pair-hopping term is switched on. At $V\sim 0.55t$ the spin velocity of the PH model reaches a maximum and then decreases to zero. A similar behavior is recovered for both models at approximately $V>1.5$. In order to understand whether this surprising result has something to do with the existence of a gapless phase we have computed the spin gaps for larger systems using a DMRG approach with periodic boundary conditions. Extracting from the spin gaps some effective spin velocity (meaningful only when correlation lengths are much larger than lattice sizes) we have, here also, systematically obtained larger spin velocities for the PH model. In contrast, in the case of the Hubbard model the spin velocities are rather constant and are close to the free fermion value at small coupling. However, a remarkable result is that the abnormally large values of u_σ for the PH model tend to disappear when sufficiently accurate representations of the ground state of the system are considered (large number of states kept for the density matrix). Accordingly, our results are consistent with the fact that the unconventional behavior of spin excitations of the PH model is a transient effect specific to this model.

Now, it is quite interesting to discuss our results within the renormalization-group framework. As discussed very recently by Sikkema and Affleck, contradictory results have been reported from the RG analyses of the phase diagram of the PH model. Using standard notations (see Ref. 13), to cubic order, the RG equations for the four coupling constants of the continuum-limit Hamiltonian are

$$\begin{aligned}
-\frac{dg_s}{dl} &= g_s^2+\tfrac{1}{2}(g_s+g_4)g_s^2,\\
-\frac{dg_\rho}{dl} &= g_3^2+\tfrac{1}{2}(g_\rho-g_4)g_3^2,\\
-\frac{dg_3}{dl} &= g_\rho g_3+\tfrac{1}{4}(g_\rho^2+g_3^2-2g_\rho g_4)g_3,\\
-\frac{dg_4}{dl} &= \tfrac{3}{4}(g_\rho g_3^2-g_s^3),
\end{aligned} \tag{5.1}$$

where $l=-\ln\Lambda$, Λ being the ultraviolet cutoff. It is important to emphasize that these equations are identical for both models. The only difference lies in the initial values of the coupling constants. To the lowest-order weak-coupling limit the initial values are

$$\begin{aligned}
v_F &= 2tg_\rho=-g_s=g_3=g_4\\
&= 2V/\pi v_F \quad \text{(pair-hopping model)}
\end{aligned} \tag{5.2}$$

$$v_F=2tg_s=-g_\rho=g_3=g_4=U/\pi v_F \quad \text{(Hubbard model)}.$$

$O(V^2)$ corrections are given in Refs. 5 and 6. When solving the RG equations, a standard approach consists in considering that g_4 simply shifts the spin and charge velocities according to

$$u_\rho=v_F(1+g_4/2), \tag{5.3}$$

$$u_\sigma=v_F(1-g_4/2) \tag{5.4}$$

and then can be dropped from the RG equations. Doing this and using the initial conditions Affleck and Marston have

remarked that $g_s=0$ is not a stable fixed point and that starting with $g_s<0$ ($V>0$) then g_s flows to strong coupling, thus indicating the opening of a gap in the spin excitations. In contrast, Hui and Doniach have kept the g_4 constant in the RG equations and integrated them using the initial condition at order $O(V^2)$. By doing this they obtained that $g_s=0$ becomes a stable fixed point provided that $g_4<-2$. For $0<V/t<1$ the fixed point was obtained with $g_4\sim-2.5$. This new phase was interpreted as having no gap for single particles and spin excitations. For a full discussion of the controversy the reader is referred to Ref. 8. However, whether or not we keep the coupling constant g_4 in the RG equations, it is clear that it is difficult to draw firm conclusions using weak-coupling RG equations in a strong-coupling regime (fixed point with $g_4\sim-2.5$). Nonperturbative results are essential to support any reasonable scenario. Let us discuss our numerical results from that point of view. Figure 1 shows very clearly that the charge velocity for both models follows exactly the behavior predicted by Eqs. (5.2) and (5.3) with the correct slope. The charge degrees of freedom are gapless and the effect of the coupling constant g_4 is to renormalize the charge velocity. Figure 2 for u_σ for small sizes is consistent with the fact that a spin gap exists for the attractive Hubbard model. The behavior of u_σ is not linear at small U as would be the case for a critical system. In addition, u_σ decreases uniformly as a function of U. In contrast, as already pointed out we have found a different behavior for the PH model. At small sizes ($L=6-10$) and small coupling, u_σ is larger than the free fermion value. This is also true for larger systems ($L=14-42$) when approximate ground-state wave functions are considered. From Eqs. (5.4) we can view this regime as corresponding to a situation where the effective constant g_4 starts to renormalize to negative values. In this situation the system appears to be attracted by a fixed point similar to the one discussed by Hui and Doniach. However, as discussed before this is only a transient regime. When the low-lying eigenstates are sufficiently well described (large number of kept states in DMRG) the high-energy components responsible for this unconventional behavior are removed and the standard low-energy behavior is recovered. We believe that this very specific behavior of the PH model is at the origin of the unconventional results obtained for sizes $L=4,12$ in previous numerical works (Refs. 4, 6, and 7).

Note added in proof. Recently we became aware of a paper by A. Belkasri and F. D. Buzatu, Phys. Rev. B **53**, 7171 (1996). In this work these authors reach essentially the same conclusions as those presented here using a different method based on an approximate Bethe-Salpeter equation.

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