Phase transitions in the one-dimensional pair-hopping model: A renormalization-group study

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The phase diagram of a one-dimensional tight-binding model with a pair-hopping term (amplitude V) has been the subject of some controversy. Using two-loop renormalization-group equations and the density matrix renormalization group with lengths $L \leq 60$, we argue that no spin-gap transition occurs at half-filling for positive V, contrary to recent claims. However, we point out that away from half-filling, a *phase-separation* transition occurs at finite V. This transition and the spin-gap transition occurring at half-filling and *negative* V are analyzed numerically.

I. INTRODUCTION

In recent years interest in correlated electron systems has increased particularly in an attempt to understand high-temperature superconductors. It is important to study the effect of all possible nearest-neighbor interactions; however, the hopping of on-site spin-singlet pairs has not been well studied to date.

The Hamiltonian for the pair-hopping model is[1]

$$H = -t \sum_{\langle ij \rangle \sigma} [c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}] - V \sum_{\langle ij \rangle} [c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow} + \text{H.c.}] , \tag{1}$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (destroys) an electron of spin $\sigma = \uparrow, \downarrow$ at lattice site i, so that $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the number of electrons of spin σ at site i, and $\langle ij \rangle$ denotes nearest-neighbor pairs. Thus t and V are the single-electron- and pair-hopping amplitudes, respectively, and so this models a competition between the two hopping terms. As $t \to -t$ is a symmetry of H, in this paper we take $t \geq 0$.

At large $|V|/t$, all sites are doubly occupied or empty (assuming an even number of electrons) and the model becomes equivalent to spinless fermions.[1] In particular there is a large gap, of $\mathcal{O}(V)$, to any excited state with nonzero spin. This is true for either sign of V, but it is important to note that $V \to -V$ is *not* a symmetry of the model, unlike the Hubbard model. Finite-size numerical work[1,3] has been performed on this model in one dimension for positive V, suggesting a phase transition at which the spin gap (or single-particle excitation gap) opens, at $V/t \approx 1.4$. Two different analytical renormalization-group (RG) analyses have been applied to the model. One[2] suggested the existence of a spin gap Δ_s for all $V > 0$, with

$$\Delta_s \propto e^{-\pi t/V} \tag{2}$$

as $V/t \to 0$, and no transition for any positive V; the other[3] suggested that there is a transition at $V/t \approx 1.4$, consistent with the numerical work.

One purpose of this paper is to reexamine this question. Previous numerical work has used chains of length $L \leq 12$. We present data for much longer chains, $L \leq 60$, using White's density matrix renormalization-group (DMRG) technique[4], thereby countering the dominance of finite-size effects. We also discuss the subtleties involved in trying to extract information about the phase diagram from a low-order analytical RG calculation. Our conclusion is the same as that of Ref. 2: no phase transition for any $V > 0$.

It was argued in Ref. 2 that there *is* a phase transition, corresponding to the appearance of a spin gap, for some finite *negative* V. (The case $V < 0$ was not studied in Refs. 1 or 3.) We analyze this numerically, finding a transition at $V_c \approx -1.5t$.

There has been considerable interest of late in phase separation in the Hubbard and t-J models in one and higher dimensions. The pair-hopping model provides a simple example of a model where it is easy to see that a phase-separation transition must occur at some finite critical coupling, with a nonzero total magnetization. Consider the model at $t = 0$, with a total magnetization $M/2$, corresponding to an excess of M spin-up electrons. These electrons necessarily reside on singly occupied sites and are therefore completely immobile when $t = 0$. Thus the model is equivalent to spinless fermions with vanishing hopping terms to M sites. Equivalently we have an XY spin chain with vanishing exchange coupling to M sites, corresponding to M nonmagnetic impurities. These simply have the effect of breaking the chain up into chainlets. It is fairly clear, and can be demonstrated explicitly by a trivial calculation in the free spinless fermion

model, that the energy is lowest when all M impurities are next to each other, leaving an XY chain of $L-M$ sites. This corresponds to phase separation at $|V|/t \gg 1$ for any nonzero magnetization. On the other hand, the renormalization-group analysis of the model at weak coupling, $|V|/t \ll 1$, indicates behavior similar to that of the Hubbard model, with no phase separation. This suggests that phase-separation transitions should occur at finite values of V/t (one for positive V and one for negative V). We find evidence for such a transition at $V = V_{c1} \approx 3.5t$, but we have not examined the one at $V = V_{c2} < 0$.

In Sec. II we review and critically analyze the previous analytical RG calculations. In Sec. III we analyze quantitatively the large $|V|/t$ limit. In Sec. IV B we present our numerical work at half-filling, $M = 0$ and $V > 0$, indicating no phase transition. In Sec. IV C we present numerical evidence for the spin-gap transition at half-filling, $M = 0$ and $V < 0$. In Sec. IV D we present numerical evidence for the phase-separation transition for $M \neq 0$ at $V = V_{c1} \approx 3.5t$.

II. ANALYTICAL RG STUDIES OF THE PHASE DIAGRAM

The RG analyses of Refs. 2 and 3 came to quite different conclusions. Here we would like to explain the reasons for this and give arguments in favour of the former approach.

We use essentially the notation of Ref. 3, which is taken from the review article of Sólyom.[5] Taking the continuum limit of the pair-hopping model we obtain a general Hamiltonian

$$H = \int dx[\mathcal{H}_0 + \mathcal{H}_{\rm int}], \tag{3}$$

where $\mathcal{H}_0$ and $\mathcal{H}_{\rm int}$ are the dimensionless kinetic energy density and interaction Hamiltonian density. We keep only wave vectors close to the two Fermi points, $k \approx \pm k_F$, which we label, in position space, ψ_L and ψ_R. The kinetic energy density is given by

$$\mathcal{H}_0 = v_F \left[\psi_L^{\alpha\dagger} i \frac{d}{dx} \psi_{L\alpha} - \psi_R^{\alpha\dagger} i \frac{d}{dx} \psi_{R\alpha} \right] . \tag{4}$$

Here the spin index α is implicitly summed over; v_F is the Fermi velocity. Some of the various interaction terms can be conveniently written in terms of charge and spin currents (or densities)

$$J_L^\rho \equiv \psi_L^{\alpha\dagger} \psi_{L\alpha} \quad \text{and} \quad \vec{J}_L^s \equiv \psi_L^{\alpha\dagger} \frac{\vec{\sigma}_\alpha^\beta}{2} \psi_{L\beta}, \tag{5}$$

and similarly for J_R^ρ and $\vec{J}_R^s$. In this notation, we have

$$\begin{aligned} \mathcal{H}_{\rm int} = \pi v_F \Big\{ & -\frac{1}{2} g_\rho J_L^\rho J_R^\rho - 2 g_s \vec{J}_L^s \cdot \vec{J}_R^s \\ & - \frac{g_3}{4} [\epsilon_{\alpha\beta} \psi_L^{\alpha\dagger} \psi_L^{\beta\dagger} \epsilon^{\gamma\delta} \psi_{R\gamma} \psi_{R\delta} + (L \leftrightarrow R)] \\ & - \frac{g_4}{4} [J_L^\rho J_L^\rho - \frac{4}{3} \vec{J}_L^s \cdot \vec{J}_L^s + (L \leftrightarrow R)] \Big\} . \end{aligned} \tag{6}$$

We have chosen to write the Hamiltonian in a manifestly SU(2)-invariant way. The last term can also be written as

$$J_L^\rho J_L^\rho - \frac{4}{3} \vec{J}_L^s \cdot \vec{J}_L^s = J_L^\rho J_L^\rho - 4 J_L^{sz} J_L^{sz} = 4 J_{L\uparrow} J_{L\downarrow}, \tag{7}$$

where

$$J_{L\alpha} = \psi_L^{\alpha\dagger} \psi_{L\alpha} \text{ (repeated index not summed).} \tag{8}$$

To the first nonvanishing order in V, the bare couplings have the values

$$v_F = 2t, \quad g_\rho = -g_s = g_3 = g_4 = 2V/\pi v_F . \tag{9}$$

To cubic order, the RG equations are given by

$$\begin{aligned} -\frac{dg_s}{dl} &= g_s^2 + \tfrac{1}{2}(g_s + g_4) g_s^2 , \\ -\frac{dg_\rho}{dl} &= g_3^2 + \tfrac{1}{2}(g_\rho - g_4) g_3^2 , \\ -\frac{dg_3}{dl} &= g_\rho g_3 + \tfrac{1}{4}(g_\rho^2 + g_3^2 - 2 g_\rho g_4) g_3 , \\ -\frac{dg_4}{dl} &= \tfrac{3}{4}(g_\rho g_3^2 - g_s^3) . \end{aligned} \tag{10}$$

Here $l = -\ln \Lambda$, where Λ is an ultraviolet cutoff. As we lower the cutoff to study the long-distance behavior, l increases.

Part of the discrepancy between the conclusions of Ref. 2 and Ref. 3 arises from the treatment of the g_4 coupling. If we bosonize the theory, then

$$\begin{aligned} J_L^\rho J_L^\rho &= \frac{1}{2\pi} (\partial_+ \phi_\rho)^2 , \\ 4 J_L^{sz} J_L^{sz} &= \frac{1}{2\pi} (\partial_+ \phi_s)^2, \end{aligned} \tag{11}$$

where $\phi_{\rho,s}$ are charge and spin bosons. Hence g_4 simply shifts the velocities of charge and spin excitations to

$$\begin{aligned} v_\rho &= v_F(1 + g_4/2) , \\ v_s &= v_F(1 - g_4/2). \end{aligned} \tag{12}$$

A common approach to Luttinger liquids is to simply set v_ρ and v_s to their renormalized values and drop g_4 from the RG equations. This approach was used in Ref. 2. The RG equation for g_s then decouples from the g_ρ and g_3 ones. This arises from the fact that, upon bosonizing, the corresponding operators involve only the spin boson and only the charge boson respectively. We then see that $g_s = 0$ is not a stable fixed point: If $g_s < 0$, as is the case for $V > 0$, g_s will flow away to strong coupling. This is usually taken to indicate that the system is in a phase with a gap for spin excitations.

On the other hand, a quite different conclusion can be reached if g_4 is kept in the RG equations. Then, according to Eq. (10), $g_s = 0$ becomes a stable fixed point from the negative side provided that $g_4 < -2$. The nature of this putative phase can be understood by also rewriting the free electron kinetic energy in terms of spin and charge currents. Setting all coupling constants to zero

except g_4, the full Hamiltonian density can be written

$$\mathcal{H} = \frac{\pi v_F}{2}\left[\left(1-\frac{g_4}{2}\right)J_L^\rho J_L^\rho + \left(1+\frac{g_4}{2}\right)J_L^{sz}J_L^{sz}\right] + (L \leftrightarrow R). \tag{13}$$

We see that for $g_4 < -2$, the spin part of the Hamiltonian becomes unstable. That is, $J_L^{sz}(x)$ and $J_R^{sz}(x)$ tend to become large, necessitating the keeping of higher-order terms in the Hamiltonian. On the other hand, the condition of zero total magnetization requires

$$\int dx[J_L^{sz} + J_R^{sz}] = 0\ . \tag{14}$$

A possible interpretation of this phase (which occurs in other known cases) is a ferromagnetic phase. The condition of zero total magnetization forces a domain structure, i.e., phase separation, to occur. One side of the system has positive polarization and the other half negative.

In Ref. 3, the cubic RG equations were integrated, including g_4, using the initial values of Eq. (9) [plus the $\mathcal{O}(V^2)$ corrections which are not important at small V]. The result was that for $0 < V/t < 1$, a fixed point was reached with $g_4 \approx -2.5$ and $g_s = 0$.

Whether or not g_4 is included, for $V/t < 1$, g_3 renormalizes to a zero and g_ρ to some small positive value which depends on V/t, corresponding to a zero gap for charge excitations.

In Ref. 2 this phase was identified as having a spin gap since g_s does not flow to zero. In Ref. 3 this phase, with $g_s = 0$ and $g_4 < -2$, was assumed to have no gap for single-particle excitations. Since these excitations have spin $\frac{1}{2}$ and charge 1, this would imply, from the usual Luttinger liquid viewpoint, that there is neither a charge gap nor a spin gap. We do not find this calculation convincing. It is not possible to argue rigorously that g_4 renormalizes to a value less than -2 using only the cubic order RG equations. If this actually happened, as claimed in Ref. 3, this would presumably imply a transition into a ferromagnetic phase [or possibly some other more exotic phase characterized by the harmonic spin Hamiltonian of Eq. (13) becoming unstable] for arbitrarily small V. No direct numerical evidence for ferromagnetism (or other exotic behavior) at small V/t has been presented. Although earlier numerical work in Refs. 1 and 3 saw indications of a vanishing spin gap in this region of parameters, the numerical results presented here in Sec. IV B based on much longer chains ($L \leq 60$ instead of $L \leq 12$) find a nonzero spin gap.

In Ref. 3 a different phase is reached for $V/t > 1$ with a non-zero g_s at the fixed point, corresponding to a spin gap as in Ref. 2. However, Refs. 2 and 3 now disagree about the behavior of the charge couplings, g_ρ and g_3. Note that the second and third RG equations in Eq. (10) imply that $g_3 = \pm g_\rho$ are separatrices (for $g_4 = 0$). For $g_\rho > 0$, if $|g_3| \leq g_\rho$, g_3 flows to zero (see Fig. 1), corresponding to a harmonic gapless effective Hamiltonian for charge. Outside this region both g_3 and g_ρ flow off to values of $\mathcal{O}(1)$. This is normally interpreted as a phase with a charge gap. It is a remarkable feature of the pair-hopping model that, to $\mathcal{O}(V)$, $g_\rho = g_3$: The system lies on a separatrix. It is necessary to calculate the bare couplings to $\mathcal{O}(V^2)$ to deduce whether or not g_3 flows to zero. Both papers agree that these $\mathcal{O}(V^2)$ terms place the bare couplings in the basin of attraction of the $g_3 = 0$ critical line, for small V. In Ref. 2 it was assumed (on the grounds of simplicity) that the system remained in this basin of attraction for all $V > 0$. On the other hand, in Ref. 3, the expression for the bare couplings to $\mathcal{O}(V^2)$ was used for arbitrarily large V to deduce that the bare couplings moved outside this basin of attraction at a critical $V \approx t$ (the same critical point at which g_s and g_4 change). The cubic RG equations predict a fixed point at $g_\rho = g_3 = -2$, which the authors of Ref. 3 assume corresponds to vanishing charge gap.

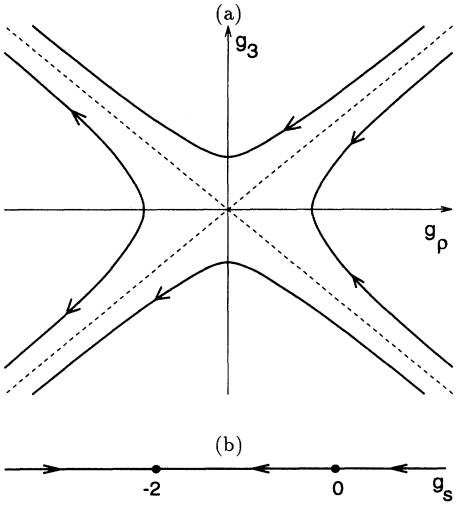

FIG. 1. Third-order RG flow diagrams, ignoring g_4. (a) Flow in the charge sector, for small g_3 and g_ρ. (b) Flow in the spin sector.

This argument concerns us because it is not possible to tell from these low-order calculations of the bare couplings and the RG equations whether or not the bare couplings ever leave the domain of attraction of the $g_3 = 0$ critical line. Furthermore, if they did, this phase would normally be identified as having a charge gap, which we know does not occur for small or large V. [The existence of an apparent, finite coupling fixed point of the cubic RG equations at couplings of $\mathcal{O}(1)$ does not necessarily signal the existence of a different critical point. It could disappear upon keeping higher-order terms.]

In Sec. III we give analytic arguments implying that, for large $|V|/t$, there is a spin gap but no charge gap.

By ignoring g_4 (i.e., absorbing it into velocity renormalizations) and making a plausible assumption about the behavior of bare coupling constants at large V, we obtain simple behavior requiring no phase transition for any $V > 0$. There is always a spin gap and no charge gap.

On the other hand,[3] by including the renormalization of g_4 and using weak coupling results at strong coupling one obtains two different phases: a bizarre small-V phase with an unstable harmonic spin Hamiltonian and a large-

V phase which would likely correspond to a charge gap, in contradiction with the expected large-V result.

The authors of Ref. 3 applied the same RG analysis to the positive-U Hubbard model. Their analysis gave a small-U phase with $g_4 > 2$, corresponding to a negative harmonic Hamiltonian in the charge sector and a large U phase with a nonzero g_s which would normally correspond to a spin gap. As they pointed out themselves, this is in contradiction with the expected behavior which is a charge gap and no spin gap for all positive U (at half-filling).

III. LARGE $|V|$ LIMIT: SPIN GAP AND PHASE SEPARATION

The pair destruction operators $a_i \equiv c_{i\downarrow}c_{i\uparrow}$ have commutation relations $[a_i, a_j^\dagger] = (1 - n_i)\delta_{ij}$, where $n_i = \sum_\sigma n_{i\sigma}$. So the a's commute if $n_i = 1$ since they have no effect on singly occupied sites. In the other two cases $n_i = 0, 2$ we have $n_i = 2a_i^\dagger a_i$ so that the a_i's are spinless fermion operators, obeying $\{a_i, a_j^\dagger\} = \delta_{ij}$. As shown in Ref. 1, setting $t = 0$ results in a ground state involving only empty and doubly occupied sites, and so the on-site pairs are effectively spinless fermions.

The DMRG method that we use requires free boundary conditions. So we analytically examine the large $|V|$ limit for an open chain, noting that nothing essential will change in going to periodic or infinite length chains. The ground state energy for an open chain of even length L is easily computed to be

$$E_0 = -2|V| \sum_{n=1}^{L/2} \cos \frac{n\pi}{L+1} = |V| \left(1 - \csc \frac{\pi}{2L+2}\right). \tag{15}$$

Adding a single electron to this half-filling ground state produces an immobile site since $t = 0$, effectively breaking the chain. The energy will depend on the location of the break, and is easily shown to be minimized if the break is at the end of the chain, in which case the energy is that of $\frac{L}{2}$ pairs hopping on an open chain of length $L - 1$, namely,

$$E_1 = -2|V| \sum_{n=1}^{L/2} \cos \frac{n\pi}{L} = |V| \left(1 - \cot \frac{\pi}{2L}\right). \tag{16}$$

So the single-particle gap for the open chain is

$$\Delta_{\rm sp} = |V| \left[\csc \frac{\pi}{2L+2} - \cot \frac{\pi}{2L}\right] \tag{17}$$

$$= |V| \left[\frac{2}{\pi} + \frac{\pi}{4L} - \frac{\pi}{12L^2} + \mathcal{O}\left(\frac{1}{L^3}\right)\right]. \tag{18}$$

So, for $t = 0$, we have a model equivalent to free spinless fermions, corresponding to a spin gap proportional to $|V|$ but no charge gap. To see whether this situation persists for finite $|V|/t$, we can do perturbation theory in the lattice model in t/V. This is very similar to the well-known results on the large-U Hubbard model. In this case we project out singly occupied sites. A single application of t takes us into the high-energy subspace with two singly occupied sites. In second-order perturbation theory we generate an effective interaction of $\mathcal{O}(t^2/V)$ in the spinless fermion model. This simply corresponds to a nearest-neighbor interaction of the spinless fermions. This interaction is known to be exactly marginal, leading to a critical line with vanishing gap.

Thus there is a spin gap for large $|V|/t$. As there is no spin (or charge) gap for $V = 0$, there must be some transition. On the basis of a reliable interpretation of the analytical RG equations and careful consideration of and comparison with numerical RG results, we conclude that the positive-V transition occurs at $V = 0$ instead of at some finite $|V|$. We show numerically that for small positive V, the behavior of the single-particle gap is of the form predicted by the RG flows (upon dropping g_4) in the numerically accessible region of phase space. We also find a spin-gap transition at $V = V_c \approx -1.5t$.

The above analysis also shows that in the case $t = 0$, a single unpaired electron sits at a chain end; it is clear that additional electrons of the same S^z will clump at the chain ends as well. That is, at finite magnetization, the chain phase separates: One part of the chain assumes the net magnetization. It is important to note that this is not a peculiarity of the open chain; in the periodic case as well, at $t = 0$, added polarized electrons cut the chain and the chain-breaking energy is clearly minimized by clumping them together. Since going from $t = 0$ to some large but finite $|V|/t$ introduces only a marginal operator, it is clear that this phase separation will persist to some critical values of V, which probably have different absolute values because the Hamiltonian is not symmetric under $V \to -V$.

IV. RESULTS OF NUMERICAL RG

A. DMRG details

We use the "infinite system DMRG method,"[4] treating open chains of even length up to 60, and maintaining 64 (sometimes 128) states in each block. The ground state has total spin 0 and is at half-filling; we add a single electron (pair of electrons of opposite spin) to compute the spin (charge) gap for each length. These results are extrapolated to infinite length taking into account truncation error uncertainties. The figures summarize the results of our DMRG calculations, as explained in this section.

B. Spin gap for $V > 0$

We find that the spin gap does not vanish for any $V > 0$, as shown in Fig. 2. In comparing its dependence on V with that predicted from the analytical RG of Ref. 2, namely,

$$\Delta_s \approx te^{-\pi t/V} \tag{19}$$

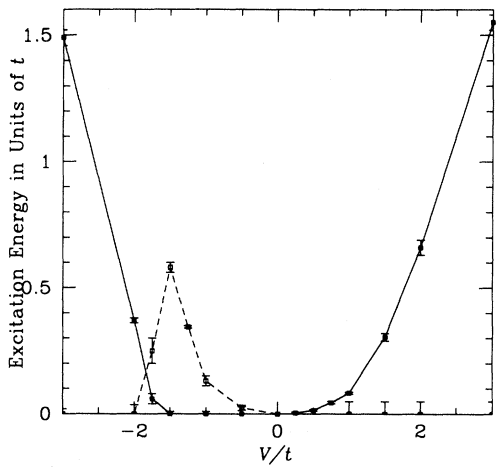

FIG. 2. Summary of numerical results: the open squares and dashed line are the charge gap, and the solid squares and solid line are the spin gap. A clear phase transition is evident near $V = V_c \approx -1.5t$, but for positive V, the spin gap opens up from $V = 0$. The error bars indicate uncertainty in extrapolating $L^{-1} \to 0$; the lines are to guide the eye.

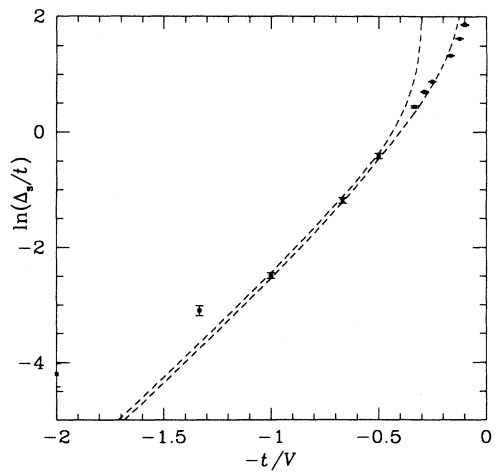

FIG. 3. Fitting the DMRG data for only two points, namely, $V/t = 1, 2$, to the form given by Eq. (22); the dashed lines are the upper and lower limits of the resulting fitted curves taking the numerical error bars into account. The lower limit extrapolates well over the range $t < V < 4t$, which is the expected region of validity. (The fit is not expected to be valid for $V < t$ because of the finite-size gap, while $V > V_{c1} \approx 3.5t$ is the phase-separated region.)

(after correcting the typographical error), which is valid for small V/t, the numerical work is not dependable for $V/t < 1$ because there the expected correlation length $\xi \approx v_F/2\Delta$ becomes of order the system size L. The finite-size gap alone is $\Delta_{FS} \approx \pi v_F/L$ so that one cannot expect to measure Δ/t lower than $\Delta_{FS}/t \approx 2\pi/L \approx 0.1$ for $L = 60$.

The RG flow equations to two-loop order, after dropping g_4 as explained in Sec. II, give for the spin coupling g_s

$$g_s^{-1} - g_{s0}^{-1} - \frac{1}{2}\ln\frac{1+2g_s^{-1}}{1+2g_{s0}^{-1}} = \ln\frac{L}{L_0}, \tag{20}$$

where L_0 is an initial length scale ($\Lambda = L^{-1}$ is the ultraviolet cutoff) and the initial spin coupling is[3]

$$g_{s0} = -\frac{V}{\pi t} + \left(\frac{V}{\pi t}\right)^2 \ln\left(\tan\frac{1}{tL_0}\right). \tag{21}$$

We take the spin gap to be the energy (inverse length) scale at which g_s enters the regime of strong coupling, specifically where $g_s = a = \mathcal{O}(-1)$, resulting in

$$\Delta_s(V) = \Delta_0 \exp(g_{s0}^{-1} - a^{-1})\sqrt{\frac{1+2a^{-1}}{1+2g_{s0}^{-1}}}, \tag{22}$$

where $a = \mathcal{O}(-1)$ is used as the criterion for $|g_s|$ becoming large. Figure 3 shows that the numerically computed spin gap is indeed of the form predicted by the RG flow equations with g_4 dropped.

While the above comparison of the RG flows are to numerical results on open (not periodic) chains, we believe these results (and in particular the nonvanishing of the gap for $V > 0$) constitute a reliable estimate of the situation in the thermodynamic limit. However, the situation is somewhat different in the phase-separated region ($V > V_{c1} \approx 3.5t$ and $V < V_{c2} < 0$) than in the non-phase-separated region at smaller $|V|$. In the non-phase-separated region, the excitation which we study is concentrated in the bulk of the chain as discussed in Sec. IV D and Figs. 4–6. Thus we expect that its excitation energy is not affected significantly by the boundary conditions for sufficiently long chains. However, in the phase-separated region, the excitation lives near the ends of the chain and its energy may well be strongly affected by the boundary conditions. In this case, the energy which we measure is still a lower bound on the bulk gap. This follows because the state which we study is the lowest-energy one with these quantum numbers. If the bulk gap were lower, we would expect a lower-energy state to exist, localized far from the chain ends. Thus our results give strong evidence for a spin gap for all $V > 0$ but only give a reliable estimate of the size of the gap for $V_{c2} < V < V_{c1} \approx 3.5t$, except for magnitudes less than the finite-size gap as discussed above.

C. Phase transition at $V = V_c \approx -1.5t$

As discussed in Ref. 2, for small $V < 0$ the pair-hopping model is identical to the positive-U Hubbard model. Thus we expect a charge gap but no spin gap in this region. It was also argued that there should be a phase transition at finite $V < 0$ because at $V/t \to -\infty$ there is no charge gap but a spin gap. In Fig. 2 we present DMRG results confirming this prediction, with the transition occurring at $V = V_c \approx -1.5t$. Our numerical results are consistent with the spin gap appearing at the same critical coupling at which the charge gap disappears; however, the presence of two distinct critical

couplings cannot be ruled out. It is unclear to us whether this critical point (or points) simply corresponds to the renormalized couplings g_s and g_3 passing through zero or to some more exotic critical point.

D. Phase separation at $V = V_{c1} \approx 3.5t$

To demonstrate the phase-separation transition, we examine the behavior of wave functions obtained using the DMRG at $L = 60$ in the sector of one electron added relative to half-filling. Specifically, we plot in Fig. 4 the expectation value of $S^z(i)$ for sites $i = 1, \ldots, 30$ (the chain is symmetric about the central link) for different values of V/t. For large V, the excess spin is localized at the chain ends, and as V is reduced, the spin extends further into the bulk. As V/t drops from 4 to 3, looking at the wave function near the center of the chain shows that near these values of V/t the spin becomes unbound from the chain end and is rapidly and fully delocalized into the bulk of the chain, leading us to consider $V_{c1} \approx 3.5t$ as a phase-separation critical point. This conclusion is further verified by examining the spin on the chain end as a function of V/t, as well as the total spin in the centre half of the chain, as shown in Figs. 5 and 6.

Due to the fact that we have employed the infinite system method, instead of the finite system method,[4] these wave functions are not expected to be precise particularly near the phase-separation transition and at the chain ends. However, we expect that the results are accurate to within a few percent at worst, certainly not affecting the qualitative behavior of our figures which clearly demonstrate the phase-separation transition.

While *a priori* this phase transition could occur at a different value of V than the bulk phase separation, the simplest scenario would have both transitions occurring at the same point: Essentially the bulk transition drives the boundary transition. The numerical evidence on one and two added electrons seems to indicate that for low net magnetization, V_{c1} is constant.

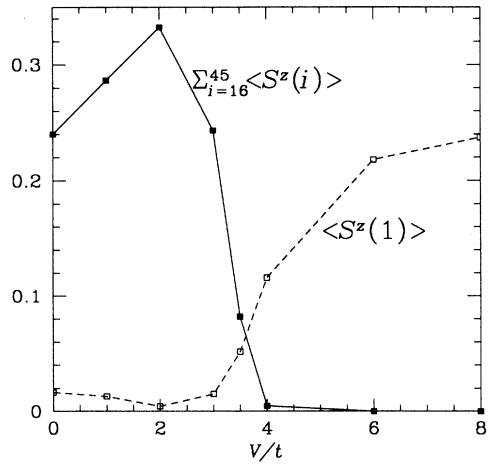

FIG. 5. Spin at a chain end (open squares) and net spin in the center half of the chain (solid squares) as a function of V/t for a single added electron.

This phase-separation transition will occur for finite V_{c1} in the periodic and infinite chain as well (though not necessarily at the same value of V_{c1} as for the open chain): Added unpaired electrons will still break the chain into chainlets and the energy will be minimized if they clump together. However, it will be more difficult to detect in a periodic chain since the ground state is usually translationally invariant.

V. CONCLUSIONS

We conclude that there is a finite spin gap for all positive V in the half-filled pair-hopping model in one di-

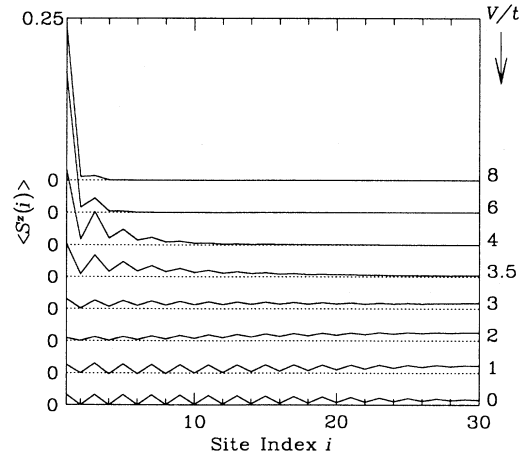

FIG. 4. Expectation values $\langle S^z(i) \rangle$ for for different values of V/t, for one electron added relative to half-filling. The unpaired electron delocalizes into the chain near $V/t = 3.5$. (The $L = 60$ chain is symmetric about its central link.)

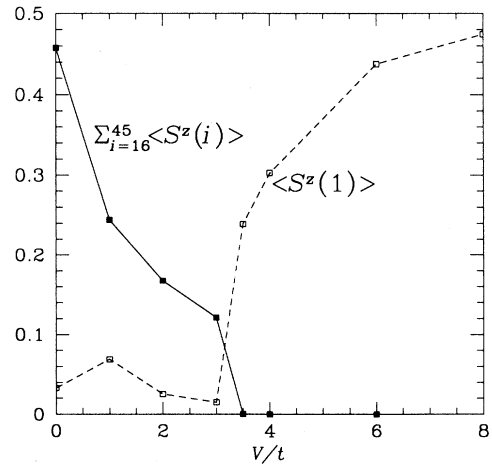

FIG. 6. Spin at a chain end (open squares) and net spin in the centre half of the chain (solid squares) as a function of V/t for two added electrons.

mension, and that to accurately describe its behavior as a function of V, one must neglect the coupling g_4 in the renormalization-group flows.

We conclude that there are phase-separation transitions in the pair-hopping model, one at positive V and one at negative V. In one dimension at low doping from half-filling, for $V > V_{c1} \approx 3.5t$ polarized electrons clump together.

We conclude that there is a new critical point at (or possibly two critical points near) $V = V_c \approx -1.5t$ at which, proceeding from weak coupling, a spin gap opens and the charge gap closes at half-filling.

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