Phase separation in \( t-J \) ladders

Stefan Rommer and Steven R. White
Department of Physics and Astronomy, University of California, Irvine, California 92697

D. J. Scalapino
Department of Physics, University of California, Santa Barbara, California 93106
(Received 27 December 1999)

The phase separation boundary of isotropic \( t-J \) ladders is analyzed using density matrix renormalization group techniques. The complete boundary to phase separation as a function of \( J/t \) and doping is determined for a chain and for ladders with two, three, and four legs. Six-chain ladders have been analyzed at low hole doping. We use a direct approach in which the phase separation boundary is determined by measuring the hole density in the part of the system which contains both electrons and holes. In addition, we examine the binding energy of multihole clusters. An extrapolation in the number of legs suggests that the lowest \( J/t \) for phase separation to occur in the two-dimensional \( t-J \) model is \( J/t \sim 1 \).

I. INTRODUCTION

Phase separation in strongly correlated electron systems doped with holes and its connection to high-temperature superconductivity has attracted much attention in the last ten years. Experimental evidence for phase separation\(^1\) found in \( \text{La}_2\text{CuO}_4 \) and the desire to understand the full phase diagram of strongly correlated models have led to intensive studies of this effect in the \( t-J \) and Hubbard models. The \( t-J \) model is one of the most basic models describing mobile holes in an antiferromagnetic background. Nevertheless, there is currently no general agreement for the phase separation (PS) boundary of the two-dimensional (2D) \( t-J \) model. At large interaction strengths \( J/t \) the segregation of the system into an antiferromagnetic region without holes and a hole-rich region is well established. What happens in the physically relevant region for smaller \( J/t \) values and near half filling is, however, controversial.

Emery, Kivelson, and Lin suggested that the 2D \( t-J \) model phase separates at all interaction strengths close to half filling based on variational arguments and exact diagonalization of \( 4 \times 4 \) clusters.\(^2\) Later Putikka, Luchini, and Rice found phase separation only for \( J/t > 1.2 \) using a high-temperature expansion.\(^3\) Dagotto et al. diagonalized \( 4 \times 4 \) clusters and came to a similar conclusion.\(^4\) They argued that at small \( J/t \) there is a region where holes bind into pairs but that PS starts only at \( J/t \sim 1 \). Variational calculations and numerical studies on larger lattices by other authors have also yielded similar results.\(^5-9\)

More recently Hellberg and Manousakis used a Green’s function Monte Carlo technique and found results in agreement with Emery et al., i.e., PS at all interaction strengths close to half filling.\(^10\) On the other hand, subsequently Calandra, Becca, and Sorella used Green’s function Monte Carlo and found evidence for PS only for \( J/t > 0.4 \).\(^11\) White and Scalapino concluded in a comparison of density matrix renormalization group (DMRG) results and other numerical results by different authors that the ground state at small \( J/t \) close to half filling should be striped and not phase separated.\(^12\)

In this paper we use DMRG techniques\(^13\) to numerically study \( t-J \) ladders with up to six chains and determine the phase separation boundary as a function of interaction strength and doping. This paper approaches the problem from a different direction than previous studies. DMRG is highly accurate for narrow ladder systems, so here we determine precise phase boundaries for narrow ladders and then consider what happens as the ladders are made wider. As we will show in the next section we find that an extrapolation in the width of the ladder systems favors a lowest interaction strength of \( J/t \sim 1 \) for phase separation to occur in a 2D system.

Apart from being important to study the role of dimensionality on physical properties and to give insight into 2D systems, ladder systems are very interesting in their own right, since they can be realized in various materials. For example, it has been found that \( \text{La}_{1-x}\text{Sr}_x\text{CuO}_2 \) consists of two chain ladders\(^15\) while \( \text{Sr}_{2n-2}\text{Cu}_n\text{O}_{4n-2} \) has \( n \)-leg ladders weakly coupled to each other.\(^14\) Another example of a multiladder compound is \( \text{La}_{4-4x}\text{Cu}_8\text{O}_{16+8x} \).\(^16\)

The rest of this paper is organized as follows. In Sec. II, before going into any details on our numerics and results, we present our main findings for the phase separation boundary. In Sec. III we present the model and the methods we have used. Section IV contains the detailed results and in Sec. V we summarize and conclude.

II. PHASE BOUNDARY

Leaving the details to a later section, we present the main result here. The phase boundary for one-, two-, three-, and four-leg ladders is shown in Fig. 1. For the six-chain ladders we have determined the PS boundary at low hole doping as is indicated in the figure. A detailed discussion of the method we have used to obtain the phase separation boundary and the results for each ladder are given in Sec. IV.

The DMRG has proven to be an accurate method for studying one-dimensional systems and ladder systems of limited width. The results presented in Fig. 1 and in Sec. IV for systems with up to six legs should be very reliable and...
III. MODEL AND METHOD

The Hamiltonian of the $t$-$J$ model is

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.}) + J \sum_{\langle i,j \rangle} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right),$$

with the constraint of no doubly occupied sites and where $\langle i,j \rangle$ denotes nearest-neighbor sites, $\sigma (= \uparrow$ or $\downarrow$) is a spin index, $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) is the electron creation (annihilation) operator for an electron at site $i$ with spin $\sigma$, $\mathbf{S}_i = c_{i,\uparrow}^\dagger \sigma_{\uparrow} c_{i,\downarrow}$, is the spin-1/2 operator, and $n_i = \sum_{\sigma} c_{i,\sigma}^\dagger c_{i,\sigma}$. The nearest-neighbor hopping interaction is $t$ and the nearest-neighbor exchange interaction is $J$. We consider ladders with equal couplings along the legs and the rungs.

At half filling the $t$-$J$ model is equivalent to the Heisenberg model. When holes are added to the system antiferromagnetic links are removed and this increases the energy. To reduce the number of broken antiferromagnetic bonds the holes prefer to stay close together, and this can result in a phase-separated system. The kinetic part of the Hamiltonian would, however, prefer the holes to spread out, and this competition between the kinetic and exchange energy results in a rich phase diagram.

In a $t$-$J$ ladder with two or more legs, the phase-separated system consists of one region containing holes and one region without any holes. For a phase-separated system with a given $J/t$ and hole doping $x$, the density of holes in the hole-rich region gives us a point on the phase boundary curve separating phase separated and uniform systems. Using a Maxwell construction, this can easily be realized by examining the energy per site of the lowest energy uniform state as a function of the hole doping, $e(x)$, where $x$ is the total hole doping of the system. Without any holes this energy will be that of the Heisenberg model $e(x=0) = e_H$. Now consider a straight line connecting $e(x)$ between the Heisenberg point, $x=0$, and some finite doping, $x_{ps}$,

$$e_{\text{lin}}(x) = e_H + x \frac{e(x_{ps}) - e_H}{x_{ps}}.$$  

If at some doping $x$, where $0<x<x_{ps}$, we have

$$e_{\text{lin}}(x) < e(x),$$

it is possible for the uniform system to lower its energy by forming two separate phases, one with hole density $x_{ps}$ and one with no holes. The inequality (3) will be fulfilled when $e(x)$ has a negative second derivative. In this case the density of the hole-rich region, $x_{ps}$, is found by minimizing Eq. (2) with respect to $x_{ps}$. It is easily shown that this corresponds to an $x_{ps}$ such that the slope of $e(x)$ at $x_{ps}$ is equal to the slope of the straight line $e_{\text{lin}}(x)$.

For large enough value of $J/t$, we have a fully phase-separated system with $x_{ps}=1$. In this case the system consists of a Heisenberg ($x=0$) region and a completely electron-free ($x=1$) region.

For a single chain at large enough $J/t$ the situation is the same: the system is fully phase separated and has a Heisenberg phase and an empty phase. However, at intermediate values of $J/t$ the chain and the ladders are quite different. If we reduce $J/t$ for the ladders or for a two-dimensional system, the empty phase becomes unstable first and electron pairs evaporate into the electron-free region. However, as we reduce $J/t$ in a single chain it is the Heisenberg phase that gets destroyed first and holes evaporate into this hole-free region. This means that for an intermediate range of $J/t$ the chain has one region without any electrons and one region with electrons and holes. This is seen in Fig. 1 where

FIG. 1. Boundary to phase-separated region where $\langle n_x \rangle$ is the total electron density of the system. Phase separation is realized to the right of the curves.

thus settle the issue of the phase boundary for these ladders. What is less clear is whether, knowing that the result for each ladder is accurate, it is possible to find the behavior of a 2D system by doing an extrapolation in the number of legs.

Since the controversy about 2D systems has primarily been about the PS boundary close to half filling, we will focus on the critical $J/t$ value for phase separation for $\langle n_x \rangle = 1$, where $\langle n_x \rangle$ is the average electron density. We can get an estimate for the 2D model by extrapolating our data in the number of legs as shown in Fig. 2. We find the PS boundary at about $J/t \approx 1$. From our data we cannot tell the exact functional form of the convergence to 2D. However, as can be seen in Fig. 2, the qualitative conclusion made above does not depend on whether the convergence is linear or quadratic in the inverse number of legs.

FIG. 2. Phase-separation boundary at low hole doping as a function of the inverse number of legs. The arrow indicates $J/t \approx 0.35$, a typical value of $J/t$ for the cuprates.
the PS boundary for a chain occurs at a smaller $J/t$ at low electron density than at low hole doping while the opposite is true for the ladders.

For chains as with the ladders, the density of holes in the mixed phase (containing both electrons and holes) is equal to the boundary density at which phase separation sets in. Thus, by determining the hole density in the hole-rich region we automatically know the PS boundary. The problem of mapping out the boundary line in the two-dimensional $(J/t, x)$ space is then reduced to a one-dimensional problem: for each $J/t$ we get one point on the PS boundary (as long as the system is phase separated). Using DMRG we can determine the PS boundary in a very direct way by actually measuring the hole density in the mixed phase.

The initial positions of the holes are determined during the DMRG system buildup sweep by choosing appropriate quantum numbers for the target state in each iteration. After this sweep a number of finite size sweeps are done. Starting with a uniform hole distribution and letting a possible phase-separated state form during the finite size sweeps is a possible but rather slowly converging method. It is better to distribute the holes uniformly in only part of the system and let the DMRG converge from there. By doing several runs for the same hole doping and $J/t$, each time adjusting the initial hole configuration according to the previous results in a self consistent fashion, it is possible to speed up convergence. When the DMRG has converged we measure the total hole density in the rungs,

$$n_A\langle l_x, l_y \rangle = \sum_{l_y} \left[ 1 - \sum_{x} \langle c_{l_x, l_y, x}^\dagger c_{l_x, l_y, x} \rangle \right],$$

and determine $x_{\text{ps}}$. Here $c_{l_x, l_y, x}$ is the electron annihilation operator at site $(l_x, l_y)$.

At very low hole doping it becomes more difficult for the DMRG to converge to a uniform density of holes in the hole-rich phase. To estimate the PS boundary at low hole doping we therefore also consider the binding of holes. At intermediate couplings $J/t$ the holes bind to form many-hole bound states (pairs and domain walls) as will be discussed in more detail for each ladder system below. The binding energy of two domain walls (stripes) with $h$ holes each is defined by

$$E_b(h) = 2(E_h - E_0) - (2E_h - E_0),$$

where $E_h$ is the ground state energy of a system with $h$ holes. For couplings such that a $2h$-hole compound breaks up into two $h$-hole stripes the binding energy is zero. With only a few holes in a bound state located around the center of the ladder we have been able to use long enough ladders so that the holes are always far from the open boundaries at the ends of the legs. The binding energy in Eq. (5) is then nearly independent of the system length. By determining the coupling $J/t$ at which the $2h$-hole complex breaks apart, i.e., where $E_b = 0$, we find an estimate for the PS boundary in the limit of low hole doping.

There is of course the possibility that the binding of two stripes does not signal phase separation but instead corresponds to the formation of another state with twice as many holes in each stripe. By comparing the estimates for the PS boundary for finite hole density determined by measuring the density in the hole-rich phase as described above with estimates from the binding of stripes we find that the two results agree well at low hole doping. We thus believe that this does not occur. Another exotic possibility is that a striped state is not uniformly striped but actually phase separated into a striped phase with a fixed, fairly large spacing between stripes and a Heisenberg phase. We have not seen indications for such a phase in our calculations. However, if this were to occur at very low hole doping (say $x \sim 0.01$) we would not be able to detect it, particularly on the wider ladders. We believe that our method of calculating the PS boundary value $J/t$ is a more accurate method than estimating $x_{\text{ps}}$ by a minimization of $e_{\text{ps}}(x)$, especially at low hole doping where the minimum occurs very close to the Heisenberg point $x = 0$.

Since the DMRG is most accurate for systems with open boundary conditions we have used open boundary conditions (BC) in the leg direction. We have, however, performed calculations on several system lengths to examine the effects of the open edges. For the ladders with four legs or less we were able to treat long enough systems to make finite length effects negligible. For the six-chain ladder we were more limited in length but we still believe our results to be accurate.

For the two-, three-, and four-chain ladders we have used open boundary conditions also in the rung direction. It has been found that three- and four-hole stripes form in the rung direction on the open three- and four-leg ladders, respectively. Macroscopic phase separation, which can be viewed as the attraction and binding of stripes, can thus be naturally studied in these systems. We have further found that stripes in the rung direction form in six-leg ladders with cylindrical boundary conditions, i.e., periodic BC in the rung direction. On the other hand, in open six-chain ladders with reasonably large $J/t$ the holes localize on the four outermost legs. This situation leaves the two middle legs essentially hole-free, at least partly because only three antiferromagnetic bonds will be broken if a hole is positioned at an open boundary compared to four broken bonds for a hole in the bulk. Therefore we used cylindrical BC with all six-chain ladders studied in this article. The open three- and four-leg ladders only have sites that are either at a boundary or next to a boundary, and the hole density variations in a rung are therefore expected to be smaller than those in the six-chain systems. In fact, for the three- and four-leg systems near and in the phase-separated region we always found many-hole complexes that were essentially uniform in the rung direction even with open BC. Furthermore, three- and four-leg systems with cylindrical BC can have strong finite size effects stemming from frustration in the short transverse direction. Therefore, we did not consider three- and four-leg systems with cylindrical boundary conditions.

We keep at most 2400 states in our DMRG calculations and the truncation errors range from less than $10^{-7}$ for the single chain to less than $10^{-4}$ for the six-chain ladder. To reduce effects from the open boundaries at the ends of the legs we sometimes apply a small local chemical potential at the outermost rungs. This reduces the attraction of holes to the edges and makes the hole density close to the edges...
smoother. A local chemical potential between $\mu \approx 0.2(J/t)$ and $\mu \approx 0.5(J/t)$ was typically used.

IV. RESULTS

A. One chain

We first consider the simplest case, a single chain with open boundary conditions. The hole density along the chain for three values of $J/t$ is shown in Fig. 3. As can be seen, the system separates into an electron-free region and a region with both holes and electrons. By measuring the hole density in the mixed region for a given $J/t$ we directly find the phase separation boundary $x_{ps}$ as discussed in the previous section. The complete phase-separation boundary is plotted in Fig. 1. Our results agree well with the results at intermediate doping by Ogata et al.,17 but they did not determine the phase boundary at very low hole doping or very low electron densities. We also find reasonable agreement with the results of Hellberg and Mele,20 although there are small differences at low and high dopings. However, we believe our results for a single chain are more accurate than previous studies.

B. Two chains

We next consider a two-chain ladder with open boundary conditions. Some of the data for the two chain systems shown here were originally presented in Ref. 21, where it was found that a recurrent variational ansatz gave qualitatively similar results. Here we present additional results and explain the calculational technique in more detail. We have calculated the hole density for $80 \times 2$ systems at different coupling parameters $J/t$. The total hole density in the rungs, as defined in Eq. 4, is shown in Fig. 4 for three values of $J/t$. As seen the system now divides into a hole-free region and a mixed region.

For $J/t$ just smaller than where the model phase separates we find that four-hole clusters split up into two pairs but that pairs are stable. Inside the phase-separated phase the four-hole clusters of course are stable and we have determined the binding energy of two pairs, $E_b(2)$, as defined in Eq. 5. The binding energies of two pairs on $32 \times 2$, $64 \times 2$, and $80 \times 2$ ladders are shown in Fig. 5. The extrapolated value at zero binding energy for the $80 \times 2$ system is $J/t \approx 2.156$. With only two or four holes located close to the center of a long lattice the energy per hole should hardly be affected by the finite size. The calculations on the different lattices in Fig. 5 support this. The value of $J/t$ where the binding energy becomes zero is thus an estimate of the PS boundary in the limit of zero hole doping, assuming that there is no intermediate phase where four holes bind but the system does not phase separate. The boundary value $J/t \approx 2.15$ does, however, connect smoothly with the boundary at larger hole doping (see Fig. 1) and we therefore exclude the possibility of a non phase separated phase with four-hole bound states.

Our results for the PS boundary agree well at low hole doping with the results of Refs. 22 and 23 although they find...
a slightly larger $J/t$ at larger dopings. This might be attributed to their method of using the divergence of the compressibility as a signature of the onset of phase separation. This criterion has been shown to give a slightly larger value of $J/t$ at the PS boundary for finite systems.\cite{10} Again, for the two-chain case we believe our results are the most accurate to date.

### C. Three chains

We now consider a three-chain ladder with open boundary conditions. We have determined the phase separation boundary by calculating the hole density of a $40 \times 3$ system at different dopings. The hole density in the rungs of three such systems is shown in Fig. 6.

The ground state properties of this system at $J/t=0.35$ has been studied by White and Scalapino.\cite{18} It was found that at low hole doping the holes form a dilute gas of uniform density. At higher doping the holes were found to bind into three-hole domain walls.

We find that just outside the PS boundary a six-hole cluster splits up into two stable three-hole domain walls. To make an estimate of the PS boundary at low hole doping we calculated the binding energy of two three-hole domain walls. Figure 7 shows the binding energy for $48 \times 3$, $64 \times 3$, and $80 \times 3$ systems. The extrapolated value at zero binding energy for the $80 \times 3$ lattice, $J \approx 1.79$, connects smoothly with the estimates at larger hole density. Many-hole bound states with more than three holes were thus not considered. The complete PS boundary line is plotted in Fig. 1.

### D. Four chains

We next consider a four-chain ladder with open boundary conditions. We have determined the phase separation boundary by measuring the hole density in the hole-rich phase of a phase separated $28 \times 4$ system. The density in the rungs in three systems is shown in Fig. 8.

White and Scalapino have found that, depending on $J/t$ and the hole doping, the ground state of this system is a state containing a dilute gas of hole pairs, a striped charge density wave domain-wall state or a phase-separated state.\cite{19} We find that just outside the PS region an eight-hole cluster is unstable and splits up into two stable four-hole domain walls. We have calculated the binding energy of two four-hole domain walls inside the PS region on $24 \times 4$, $32 \times 4$, and $48 \times 4$ lattices. The result is shown in Fig. 9. The extrapolated value at zero binding energy, $J/t \approx 1.55 \pm 0.05$, is (again) an estimate for the phase-separation boundary in the limit of small hole doping. Non-phase-separated states with bound states of more than four holes were not considered. The whole phase-separation boundary for four chains is shown in Fig. 1.

As a complement to Fig. 9 the energy per hole of different size clusters is shown in Fig. 10. For $J/t$ slightly smaller than 1.6 the eight-hole cluster splits up into two four-hole clusters

\[ \frac{E_h}{N} = \frac{1}{2} J^2 [1 - 1.9(1 - J/t)^{1/2}] \]

FIG. 8. Density of holes in the rungs of a $28 \times 4$ system for three values of $J/t$.

FIG. 9. Binding energy of two four-hole stripes in $24 \times 4$, $32 \times 4$, and $48 \times 4$ systems. The binding energy becomes zero at $J/t \approx 1.55 \pm 0.05$.

FIG. 10. Energy per hole in a $24 \times 4$ system. Error bars are of the same size as the symbols or smaller. Note that the energies have been shifted by $-1.9(1 - J/t - 1.5)$ to increase clarity of the figure. Phase separation occurs for $J/t \geq 1.55$.
that, when well separated, become degenerate in the energy per hole with a single four-hole cluster. As can be seen the four-hole bound states are preferred over pairs just outside the PS region.

E. Six chains

We next consider a six-chain ladder with periodic boundary conditions in the rung direction. Here, we find that at low hole doping and in the range of \( J/t \) studied, \( 0.6 < J/t < 2.3 \), the ground state of this system was either a state containing domain walls with four holes, domain walls with six holes, or a phase-separated state. The energy per hole in a 12 \( \times 6 \) system with different numbers of holes located around the central rungs is shown in Fig. 11. We believe that the region where a twelve hole compound has lower energy per hole than a six-hole compound is phase separated. There is thus a region with six-hole domain walls between the phase-separated region and the region with four-hole domain walls.

In the intermediate region \( 0.9 < J/t < 1.4 \), where the six-hole domain has the lowest energy per hole, a twelve-hole compound should be unstable and break up into two six-hole compounds. In Fig. 12 the hole density in three intermediate finite size sweeps from one DMRG calculation with \( J/t = 1 \) is shown. As the DMRG sweeps through the lattice, local changes in the approximation of the ground state wave function are done to minimize its energy. In the first sweep all holes were located in the center of the system but to reduce the energy they split into two six-hole stripes. A similar run with \( J/t = 0.6 \) results in a split of the twelve holes into three four-hole stripes (not shown) in agreement with Fig. 11.

To estimate the phase-separation boundary at low hole doping we have calculated the binding energy of two six-hole stripes in 8 \( \times 6 \), 10 \( \times 6 \), and 12 \( \times 6 \) systems as shown in Fig. 13. The extrapolated value at which the binding energy crosses zero is \( J/t \approx 1.4 \pm 0.2 \).

V. SUMMARY

In this paper we have studied phase separation in \( t-J \) ladders with one, two, three, four, and six legs. We have

\[
\begin{array}{|c|c|c|}
\hline
L_y & BC & J_c/t \text{ for } n_e = 1 & J_c/t \text{ for } n_e = 0 \\
\hline
1 & OBC & 3.415(2) & 2.96(1) \\
2 & OBC & 2.156(2) & 3.327(1) \\
3 & OBC & 1.79(2) & 3.51(1) \\
4 & OBC & 1.55(5) & 3.58(1) \\
6 & PBC & 1.4(2) & 3.25(5) \\
\hline
\end{array}
\]

In this paper we have studied phase separation in \( t-J \) ladders with one, two, three, four, and six legs. We have...
mapped out the complete phase-separation boundary as a function of interaction strength $J/t$ and doping. We have used a direct approach by actually calculating the density of holes in the mixed phase. At very low hole doping there are few holes in the system, and this approach becomes difficult. In this case we have estimated the phase-separation boundary by calculating the binding energy of stable many-hole complexes. In this case, extrapolation to zero binding energy gives us the estimate for the PS boundary. The critical $J/t$ for half filling and zero electron density are shown in Table I.

To investigate the possibility of a lowest limit on $J/t$ for phase separation to occur in a 2D system we made an extrapolation in the number of legs. This extrapolation suggests that the 2D $t$-$J$ model only phase separates for $J/t \approx 1$, in agreement with several previous studies.

**ACKNOWLEDGMENTS**

S. Rommer is thankful for support from the Swedish Foundation for International Cooperation in Research and Higher Education (STINT). S.R. White acknowledges support from the NSF under Grant No. DMR98-70930, and D.J. Scalapino acknowledges support from the NSF under Grant No. DMR98-17242.

\[12\] S.R. White and D.J. Scalapino, cond-mat/9907375.