Phase Separation of the Two-Dimensional $t - J$ model

C.T. Shih$^1$, Y.C. Chen$^2$, and T.K. Lee$^3$

$^1$Dept. of Physics, National Tsing Hua Univ., Hsinchu, Taiwan
$^2$Dept. of Physics, Tunghai Univ., Taichung, Taiwan
$^3$Inst. of Physics, Academia Sinica, Nankang, Taipei, Taiwan

(April 18, 2018)

The boundary of phase separation of the two-dimensional $t - J$ model is investigated by the power-Lanczos method and Maxwell construction. The method is similar to a variational approach and it determines the lower bound of the phase separation boundary with $J/t = 0.6 \pm 0.1$ in the limit $n_e \sim 1$. In the physical interesting regime of high $T_c$ superconductors where $0.3 < J/t < 0.5$ there is no phase separation.

PACS numbers: 74.20.-z, 71.27.+a, 74.25.Dw

It is believed that the main physical properties of the high-temperature superconductors can be described by the two-dimensional (2D) $t - J$ model on a square lattice. The Hamiltonian is:

$$H = -t \sum_{<i,j>\sigma} (\hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + h.c.) + J \sum_{<i,j>} (S_i \cdot S_j - \frac{1}{4} n_i n_j),$$

where $<i,j>$ is the nearest-neighbor pairs and $\hat{c}_{i\sigma} = c_{i\sigma}(1 - n_{i,-\sigma})$. In this model the two terms compete with each other. The kinetic term favors the phase which the electrons are homogeneously distributed in the plane to minimize the kinetic energy. While the exchange term attracts the electrons together to lower the magnetic energy. It is easy to see that for very large $J/t$ the system will phase separate into a hole-rich region and a region without holes to maximize the magnetic energy gain.

There are experimental evidences as well as theoretical studies that indicate phase separation and superconductivity are closely related. It is even argued that the driving mechanism of superconductivity is the same as that of phase separation or superconductivity comes from the frustrated phase separation. Hence it is extremely important to determine the phase separation boundary of the 2D $t - J$ model to resolve these issues. This paper reports our findings of the phase separation boundary.

Experimentally, phase separation of the superconducting La$_2$CuO$_{4+\delta}$ compound is observed by several measurements. The compound phase separates for $0.01 \leq \delta \leq 0.06$ below $T_{ps} \approx 300K$ into the nearly stoichiometric antiferromagnetic La$_2$CuO$_{4+\delta_1}$ with $\delta_1$ less than 0.02 and Neel temperature $T_N \approx 250K$, and a metallic superconducting oxygen-rich phase La$_2$CuO$_{4+\delta_2}$ with $\delta_2 \approx 0.06$ with $T_c \approx 34K$. The Sr doped compound La$_{2-x}$Sr$_x$CuO$_{4+\delta}$ also phase separates for $x \leq 0.03$ into superconducting La$_{2-x}$Sr$_x$CuO$_{4+\delta'}$ ($\delta' \approx 0.08$) and non-superconducting La$_{2-x}$Sr$_x$CuO$_{4+\delta''}$ ($\delta'' \approx 0.00$) phases. Recent muon spin resonance and nuclear quadrupole resonance experiments on La$_{2-x}$Sr$_x$CuO$_4$ also indicate that the doped holes were inhomogeneously distributed mesoscopically and segregated into walls separating the hole-poor antiferromagnetic domains.

Theoretically, there are conflicting results. The first important paper on this issue is by Emery et al. They used the exact diagonalization (ED) to study the $4 \times 4$ cluster. Using Maxwell construction they claimed that phase separation occurs for all values of $J/t$. This result is contradictory to the later calculations by using quantum Monte Carlo (QMC) and ED on the Hubbard model, which should be consistent with the $t - J$ model for small $J/t$. Putikka et al. studied this problem using the high-temperature series expansion and found phase separation at $T=0$ for $J/t$ lying above a line extending from $J/t = 3.8$ at zero filling to $J/t = 1.2$ at half filling. Prelovšek et al. calculated the two-point and four-point density correlations using ED on clusters of size 18 and 20 sites. They found the two-hole bound state for $J/t > 0.2$. For $J/t > 1.5$ the holes form domains walls along (1,0) or (0,1) direction, and phase separate into a hole-rich and a hole-free phase for even larger $J/t > 2.5$. Hellberg et al. determined very accurately that the critical $J/t$ for phase separation at low electron density limit is $J/t = 3.4367$. Poilblanc calculated the energy of 2 and 4 holes by ED on several clusters up to 26 sites. The phase diagram includes a liquid of d-wave hole pairs for $J/t \geq 0.2$, a liquid of hole droplets (quartets) for larger $J/t \geq 0.5$, and at even larger $J/t$, an instability towards phase separation. Yokoyama et al. investigated the phase diagram by the variational Monte Carlo (VMC) method. The critical $J/t$ for phase separation at the high density limit they found is 1.5, which is consistent with Putikka et al.

Most recently Hellberg and Manousakis investigated this problem by the Green Function Monte Carlo (GFMC) method and Maxwell construction for larger clusters. Their phase diagram is similar to Emery et al. They conclude that the $t - J$ model phase separates for all values of $J/t$ in the low doping regime.

The theoretical results of different groups discussed above are consistent at the large $J/t$ and low electron density region. But unfortunately, in the interesting
The physical regime of high $T_c$ superconductors, $0.3 < J/t < 0.5$ and high electron density $0.75 < n_e < 0.95$, they are in disagreement. We have used the power-Lanczos (PL) method \cite{20,21} to obtain the best estimate of the ground state energy in this physical regime for the largest cluster (82 sites) that have been studied so far. Based on the variational argument we show that there is no phase separation in this physical regime \cite{22}.

The ground state energy of the Hamiltonian of equation (1) is calculated by using the PL method. The PL method we used is similar to the GFMC method but without using importance sampling and the fixed node approximation. The method is essentially a variational approach. Applying more powers to a trial wave function implies a better approximation of the ground state wave function. Details of the method are discussed in Ref. 22. The trial wave functions we used are the optimized Gutzwiller wave functions, resonating valence bond state (RVB) \cite{20,21}, and RVB with antiferromagnetic long range order \cite{20}. In Fig. 1(a) energy per site is plotted as a function of $n_e$ for $J/t = 0.6$ and three different densities: $n_e = 32/36$ (open circles) and $n_e = 44/50$ (full circles) $n_e = 74/82$ (open triangles). Error bar is shown only when it is larger than the symbol. We also compared our energy of $J/t = 1$ for 50/64 with the result of high-temperature series expansion \cite{23}. The best energy we get is $-1.183(2)$ while the high-temperature expansion result is $-1.20(2)$. They are well in agreement. In Fig. 1(b) we show the best energies we are able to obtain for clusters with 36, 50 and 82 sites as a function of electronic density. For comparison we also show the exact energies of 16 sites \cite{13}. Energies are little lower for the smaller clusters. For 50 and 82 sites, there seems to be a very little finite size effect. The energy per site is a fairly smooth function of density. We do not find large effect due to different Fermi surface topology in the physical regime.

To find the phase separation boundary by using Maxwell construction we are interested in the variation of the slopes in figures like Fig. 1(b). In other words we are interested in the second derivative of energy with respect to the electronic density, or the inverse compressibility. It turns out that there is a systematic variation of this quantity as the energy approaches the ground state or as the power increases in our PL method. Although in the physical regime most of our best data have not yet converged to the exact ground state, this systematic variation is enough for us to determine the lower bound of the phase separation boundary.

It is difficult to read out the slope variation from figures like Fig.1(b), as the curve is almost a straight line for $n_e > 0.85$. Therefore we shall follow Emery et al. \cite{11} by examining another quantity. In the one-dimensional $t$–$J$ model the phase separated state contains an electron-free and an electron-rich phases. However, it phase separates into a hole-free phase, i.e., the antiferromagnetic Heisenberg island, and a hole-rich phase in the two-dimensional $t$–$J$ model. Thus the energy of the phase separated state is in the form:

$$E = (N_s - N)e_H + Ne_h$$

where $N_s$ is the total number of sites and $N$ is the number of sites in the hole-rich phase. $e_H = 1.169J$ denotes the Heisenberg energy per site \cite{24}. And $e_h$ is energy per site in the uniform hole-rich phase, which is a function of the hole density in this phase $x = N_h/N$. $N_h$ is the number of holes. $E$ can be rearranged into the form:

$$E = N_s e_H + N_h e(x)$$

where

$$e(x) = [-e_H + e_h(x)]/x$$

If $e(x)$ of a particular $J/t$ has a minimum at $x = x_m$ and the hole density of the total system is smaller than $x_m$, the system will adjust the size of the hole-rich phase $N$ such that $J_m$ is equal to $N_h/N$ and it minimizes the total energy in Eq. (3). Since $N_s$, $e_H$, and $N_h$ are all constants, the total energy is minimized as $e(x)$ is minimized. Thus $x_m$ is the critical density for phase separation at this $J/t$. 

---

**FIG. 1.** (a): Typical plots of energy per site vs powers for $J/t = 0.6$, $n_e = 32/36$ (open circles) and $n_e = 44/50$ (full circles) $n_e = 74/82$ (open triangles); (b) Energy per site as a function of electronic density for $J/t = 0.6$ with different cluster sizes. Diamonds are the exact result of 16 sites. Open circles are for 36 sites and full circles are for 50 sites, both are obtained by PL$_{power=6}$. Triangles are for 82 sites with PL$_{power=4}$. 

- $e_H$ is the Heisenberg energy per site.
- $e_h$ is energy per site in the uniform hole-rich phase.
- $x$ is the hole density in this phase.
- $N_s$ is the total number of sites.
- $N$ is the number of sites in the hole-rich phase.
- $N_h$ is the number of holes.
- $E$ is the total energy.

We calculated $e(x)$ from the energy of the uniform states $e_h(x)$ by the PL method and found the minimum of $e(x)$ on $6 \times 6$, $\sqrt{50} \times \sqrt{50}$, and $\sqrt{82} \times \sqrt{82}$ clusters for several densities and $J/t$. It is very difficult to get the converged ground state energy in the physical regime due to the sign problem. After we have found the optimized wave function in the VMC calculation we used the PL method to project the trial wave function onto the ground state systematically. The PL-1 power=4 (for 82 sites) or PL-1 power=6 (for 50 and 36 sites) energy is used here as the $e_h(x)$. It is about 2 ~ 4 percent lower than the variational energy. We estimate the difference between the best PL energy is within one or two percent of the true ground state energy.

**FIG. 2.** $e(x)$ vs hole density $x$ for (a)$J/t = 0.4$, (b) $J/t = 0.6$ and (c)$J/t = 1.5$ for several powers: PL0-VMC (open circles), PL1-VMC (full circles), PL1-power=2 (open triangles), PL1-power=4 (full triangles), and PL1-power=6 (open squares). (d)$J/t = 0.4$ for close shells of different size of lattices, 74/82, 42/50, and 50/64.

$e(x)$ vs $x = 1 - n_e$ calculated on 50 sites for $J/t = 0.4$, 0.6 and 1.5 is shown in Fig.2(a)-2(c), respectively. It is interesting to note the trend of the shift of $e(x)$ with powers. For $J/t = 0.4$ (Fig.2(a)), at the VMC level, the minimum of $e(x)$ is at $x_m = 0.16$. It shifts to $x = 0.04$ (the minimum hole density we calculated for this cluster) immediately after the first order Lanczos improvement (PL1-VMC) and stays at the density up to 6 powers. For $J/t = 0.6$ (Fig.2(b)), $x_m$ shifts from $x = 0.2$ (VMC) to $x = 0.16$ (PL1-VMC) and to $x = 0.08$ (PL1-power=6) at last. For $J/t = 1.5$ (Fig.2(c)), $x_m$ shifts from $x = 0.48$ (PL1-VMC) to $x = 0.4$ (PL1-power=2) and to $x = 0.36$ (PL1-power=6) at last. It is clear that $x_m$ shifts monotonically toward a smaller value when the energy moves closer to the ground state.

We estimated the Fermi surface by calculating $e(x)$ on different lattices. For $J/t = 0.4$, $x_m$ shifts from $x = 0.48$ (PL1-VMC) to $x = 0.4$ (PL1-power=2) and to $x = 0.36$ (PL1-power=6) at last. Hence the shell effect is not important here.

**FIG. 3.** Phase separation boundary on the phase diagram of the two-dimensional $t-J$ model evaluated by ED on the $4 \times 4$ lattice[11] (open diamonds), by the high-temperature series expansion[14] (dashed line) by the GFMC method[19] (dotted line), and the PL method on 36 sites (full triangles), 50 sites (full circles), and 82 sites(full square). The phase boundary determined by the VMC method for 36 sites (open triangles) and 50 sites (open circles) are shown in the inset.

In Fig.3 we show the phase separation boundary determined by the best $x_m$. The PL1-power=6 phase boundaries of 36 sites and 50 sites are shown as full triangles and full circles, respectively. Also some of the PL1-
power=4 data of 82 sites are also shown as full squares. For \( J/t = 0.6 \) the error bars of the \( e(x) \) for \( n_e = 80/82, \ 78/82, \) and \( 76/82 \) are larger than the difference of these three \( e(x) \), thus error bars of \( x_m \) are shown in the figure near these electron densities.

The dashed line in Fig.3 is the result of high temperature series expansion [14]. Similar result is obtained by the variational study [15]. They assumed the system separates into a hole-free Heisenberg antiferromagnet and an electron-free vacuum state. This overestimates the energy required for the phase-separated state, since electrons can “evaporate” from the Heisenberg island to gain energy. Their critical \( J_e/t \approx 1.2 \) is larger than our \( J_e/t \approx 0.6 \). Similar argument was also given by Hellberg and Manousakis [19].

Our estimate of the \( J_e/t = 0.6 \pm 0.1 \) is actually a lower bound. The exact phase separation boundary should be to the right of our result in Fig.3. When we use much poorer estimate of the ground state energy as our VMC result, the phase boundary is shifted lower. This is shown in the inset of Fig.3. The VMC results of 36 sites (open triangles) and 50 sites (open circles) show a much smaller \( J_e/t \).

Another way to understand this argument of lower bound is to examine the variation of \( e(x) \) with power. In Fig.4 we show the change of \( e(x) \) between PL1-power=6 and PL0-VMC for 50 sites. The values are proportional to the area of the circles.

In summary, we determined the phase separation boundary by the PL method and Maxwell construction. We have studied various size of clusters and densities of holes. The largest cluster studied is 2 holes in an 82 site lattice. Using the variational nature of the PL method and the systematic variation of the energy as a function of hole density we conclude that the critical \( J_e/t \) for phase separation in the low hole density limit is at least \( \approx 0.6 \). There is no phase separation in the physical regime.

It should be pointed out that the result reported above are obtained by assuming the hole-rich region in the phase separated state has a uniform hole density. We have not yet considered more exotic possibilities such as the stripe phase [14, 27, 28].

We wish to thank C.S. Hellberg, H.Q. Lin and W.O. Putikka for many useful discussions. This work is partially supported by the National Science Council of Republic of China, Grant Nos. NSC 86-2811-M-007-001R & 86-2112-M-001-042T & 86-2112-M-029-001. Part of computations were performed at the National Center for High-Performance Computing in Taiwan. We are grateful for their support.

[1] E. Dagotto et al., Phys. Rev. B 49, 3548 (1994).
[2] V. J. Emery, and S. A. Kivelson, Physica C 209, 597 (1993).
[3] J. D. Jorgensen et al, Phys. Rev. B 38, 11337 (1988).
[4] P. C. Hammel et al., Phys. Rev. B 42, 6781 (1990).
[5] P. C. Hammel et al., Physica C 185-189, 105 (1991).
[6] F. C. Chou et al., Phys. Rev. B 54, 572 (1996).
[7] J. H. Cho et al., Phys. Rev. Lett. 70, 222 (1993).
[8] J. H. Cho et al., Phys. Rev. B 46, 3179 (1992).
[9] F. Borsa et al., Physica C 235-240, 1713 (1994).
[10] F. Borsa et al., Phys. Rev. B 52, 7334 (1995).
[11] V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. 64, 475 (1990).
[12] A. Moreo et al., Phys. Rev. B 43, 11442 (1991).
[13] E. Dagotto et al., Phys. Rev. B 45, 10741 (1992).
[14] W. O. Putikka et al., Phys. Rev. Lett. 68, 538 (1992).
[15] P. Prelovšek, and X. Zotos, Phys. Rev. B 47, 5984 (1993).
[16] C. S. Hellberg, and E. Manousakis, Phys. Rev. B 52, 4639 (1995).
[17] D. Poilblanc, Phys. Rev. B 52, 9201 (1995).
[18] H. Yokoyama and M. Ogata, cond-mat/9607051.
[19] C. S. Hellberg, and E. Manousakis, cond-mat/9611195.
[20] Y. C. Chen, and T. K. Lee, Phys. Rev. B 51, 6723 (1995).
[21] E. S. Heeb, and T. M. Rice, Z. Phys. B 90, 73 (1993).
[22] Similar result has been reported by M. Khono, Phys. Rev. B 55, 1435 (1997). Although he has also used the PL method, but the largest cluster he used is 50 site in the physical regime. Using the polynomial fitting of energy as a function of density, he determined the phase boundary with $J_c/t = 0.75 \pm 0.25$. This is consistent with our result obtained with a much more careful analysis.
[23] C. Gros, Phys. Rev. B 38, 931 (1988).
[24] T. K. Lee and C. T. Shih, Phys. Rev. B 55, 5983(1996).
[25] W. O. Putikka, private communication.
[26] E. Manousakis, Rev. Mod. Phys. 63, 1 (1991).
[27] H. Tsunetsugu et al., Phys. Rev. B 51, 16456 (1995).
[28] S. R. White, and D. J. Scalapino, cond-mat/9610104.