Phase Separation Based on U(1) Slave-boson Functional Integral Approach to the t-J Model

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We investigate the phase diagram of phase separation for the hole-doped two dimensional system of antiferromagnetically correlated electrons based on the U(1) slave-boson functional integral approach to the t-J model. We show that the phase separation occurs for all values of \(J/t\), that is, whether \(0 < J/t < 1\) or \(J/t > 1\) with \(J\), the Heisenberg coupling constant and \(t\), the hopping strength. This is consistent with other numerical studies of hole-doped two dimensional antiferromagnets. The phase separation in the physically interesting \(J\) region, \(0 < J/t \leq 0.4\) is examined by introducing hole-hole (holon-holon) repulsive interaction. We find from this study that with high repulsive interaction between holes the phase separation boundary tends to remain robust in this low \(J\) region, while in the high \(J\) region, \(J/t > 0.4\), the phase separation boundary tends to disappear.

One of the most interesting observations in high-\(T_c\) cuprates (superconductors) is the phase separation, which may play an important role on superconductivity. The phase separation results from a thermodynamic instability which arises from the violation of the stability condition, \(K^{-1} = n^2 \partial^2 e / \partial n^2 = n^2 \partial^2 \mu / \partial n > 0\). Here \(K\) is the compressibility; \(e\), the ground state energy per site; \(n\), the electron density; and \(\mu\), the chemical potential. Initially the phase separation instability was believed to inhibit superconductivity. Recently it draws a great attention owing to its possible connection with superconductivity based on experimental observations in high-\(T_c\) cuprate oxides.

We write the t-J Hamiltonian for the study of the hole doped systems of antiferromagnetically correlated electrons,

\[
H = -t \sum_{\langle i,j \rangle \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) + J \sum_{\langle i,j \rangle} \left( S_i \cdot S_j - n_i n_j / 4 \right),
\]

with \(S_i = 1/2 e_{\sigma \alpha}^{i} \sigma \alpha c_{i\alpha} \) and \(n_i = \sum_{\sigma} e_{\sigma \alpha}^{i} c_{i\alpha} \) where \(e_{\sigma \alpha}^{i}\) creates an electron of spin \(\sigma\) on site \(i\). Earlier, using the t-J model a possibility of phase separation in high-\(T_c\) cuprates has been brought up by Emery et al. \cite{emery1}. They predicted the existence of phase separation at all possible values of \(J/t\), that is, \(0 < J/t \leq 1\) or \(J/t > 1\) where \(J\) is the antiferromagnetic correlation strength and \(t\), the hopping integral, including the case of \(J/t < 1\). On the other hand, other numerical studies \cite{emery1} predicted the existence of phase separation only for \(J/t \geq 1\) where \(J\) value is unrealistic for the high \(T_c\) cuprates of current interest. Recently, from a Green function Monte Carlo study Hellberg and Manousakis \cite{hellberg} reported that the phase separation can occur for all values of \(J\), in agreement with the earlier exact diagonalization study of Emery et al \cite{emery1}. In the present study, by using the U(1) slave-boson functional integral method \cite{emery2, hellberg}, we obtain a phase diagram in the plane of electron density vs. \(J/t\), by using the Maxwell construction \cite{maxwell, hellberg}. If violation of the stability condition \(K^{-1} > 0\) occurs in the electron density range of \(n_1 < n_e < n_2\), where \(n_1\) is the electron density for a hole-rich phase and \(n_2\), the electron density for a hole-free phase, the system is expected to separate into two subsystems with electron densities \(n_1\) and \(n_2\) respectively. Since we are interested in the hole-doped systems of high \(T_c\) cuprate oxides, the physics can be conveniently described in terms of the hole density, \(x = 1 - n_e\). Thus we first examine the ground state energy density \(e_h(x)\) of the hole doped system as a function of hole density \(x\). For the Maxwell’s construction \cite{maxwell, hellberg} to treat a finite system, we consider a straight line which intercepts both the Heisenberg energy \(e_H = e_h(0)\) at \(x = 0\) and a curve given by \(e_h(x)\) at \(x \neq 0\). The slope of the straight line at \(x = 0\) is then given by

\[
e(x) = \frac{e_h(x) - e_H}{x}.
\]

If a minimum of \(e(x)\) is found at a hole density of \(x = x_c\) (at which the straight line intercepts tangentially the curve of \(e_h(x)\)), phase separation is expected to exist below the onset (critical) density of \(x = x_c\). As a result the energy density of the phase separated system is described by the the linear function with slope of \(e(x_c)\) in the doping range of \(0 < x < x_c\). Thus in this region the system is stabilized with its energy lower than that of the uniform phase, by forming a system composed of two subsystems: one with a hole-rich phase of the electron density of \(n_1 = 1 - x_c\) and the other with a hole-free phase of the electron density of \(n_2 = 1\).

In order to clarify how to compute the ground state energy as a function of electron or hole density we briefly discuss our earlier approach \cite{emery2} of the U(1) slave-boson representation of the t-J Hamiltonian. In this approach we introduce an additional contribution of hole-hole repulsion to the original t-J Hamiltonian,

\[
H = -t \sum_{\langle i,j \rangle \sigma} \left( f_{i\sigma} \hat{b}^\dagger_{j\sigma} f_{j\sigma} + h.c. \right) + J \sum_{\langle i,j \rangle} \left( S_i \cdot S_j - n_i n_j / 4 \right)
\]
\[ + V \sum_{(i,j)} b_i^\dagger b_j^\dagger b_j b_i - \mu_0 \sum_i \left( f_i^\dagger f_i - N_e \right) \]  

(3)

with \( S_i = 1/2 f_i^\dagger \sigma_{\alpha \beta} f_i \) and \( n_i = \sum_i f_i^\dagger f_i \). \( \mu_0 \) is the chemical potential to fix the number of electron to \( N_e \). Here the local constraint of single occupancy, \( \sum_i f_i^\dagger f_i + b_i^\dagger b_i = 1 \) is assumed. \( f_i^\dagger (f_i) \) is the spinon creation (annihilation) operator and \( b_i (b_i^\dagger) \), the holon annihilation (creation) operator. The nearest neighbor (NN) configuration of two holes is energetically more favorable than other possible configurations. This is evident from the separate inspection of the two attractive interaction terms, \( J S_i S_j \) and \( -(J/4) n_i n_j \). For the latter we write \([17]\),

\[ -J \sum_{(i,j)} \frac{n_i n_j}{4} = - \frac{J}{4} \sum_{(i,j)} \left\{ 1 - b_i^\dagger b_i - b_j^\dagger b_j + b_i^\dagger b_j b_j b_i \right\} \]

\[ = \frac{J}{2} \sum_{i\sigma} f_i^\dagger f_i + \frac{J}{2} \sum_{i} b_i^\dagger b_i - \frac{J}{4} \sum_{(i,j)} b_i^\dagger b_j^\dagger b_j b_i. \]  

(4)

where the local constraint of single occupancy is taken into account. The effective attraction between the NN holes arises from the last term of the equation above. In view of the numerical finding of excessive large binding of hole pairs \([19]\), the hole-hole repulsive interaction term (the third term in Eq. (3)) is introduced. Owing to its introduction, we are now able to examine how phase diagram boundary is affected by the variation of hole-hole repulsion interaction \( V \). Such discussion will be made later.

As a result of the Hubbard-Stratonovich transformation \([14]\) in Eq. (3), the Heisenberg exchange and the hopping terms are led to linearized terms involving the hopping order field \( \chi_{ji} = \langle 8t/3J b_i^\dagger b_j + f_i^\dagger f_i \rangle \) in association with the exchange interaction channel and the spinon singlet pairing order field \( \Delta_{ji} = \langle j_{ji} f_i \uparrow - f_j \downarrow f_i \uparrow \rangle \) in association with the pairing channel. The contribution of the direct (Hatree) channel is omitted based on the assumption of paramagnetic states for each site, i.e., \( \langle S_i \rangle = 0 \) \([17]\). Long-range antiferromagnetic fluctuations are thus ignored in this approach \([16][17]\). The resulting effective Hamiltonian is then \([17]\),

\[ H = \sum_{(i,j)} \frac{3J}{8} \left| \chi_{ji} \right|^2 + \left| \Delta_{ji} \right|^2 - \left( \frac{8t}{3J} b_i^\dagger b_j + f_i^\dagger f_i \right) \chi_{ji} - \text{h.c.} - \left( j_{ji} f_i \uparrow - f_j \downarrow f_i \uparrow \right) \Delta_{ji}^* - \text{h.c.} \]

\[ + \frac{8t^2}{3J} \sum_{(i,j)} \left( b_i^\dagger b_j \right) \left( b_i^\dagger b_j \right) - \sum_{(i,j)} \left( \frac{J}{4} - V \right) b_i^\dagger b_j b_j b_i - \left( \mu_0 - \frac{1}{4} \right) \sum_i f_i^\dagger f_i + \frac{J}{2} \sum_i b_i^\dagger b_i \]

\[ - i \sum_i \lambda_i \left( f_i^\dagger f_i \right) + b_i^\dagger b_i - 1, \]

where a Lagrange multiplier field \( \lambda_i \) is introduced to impose the local constraint of single occupancy for both the spinon and the holon. \( \lambda_i \) will be absorbed into the effective chemical potential of holon and spinon in the mean field approaches \([16]\). The quartic holon term (the second term in Eq. (3)) above \( \frac{8t^2}{3J} \sum_{(i,j)} \left( b_i^\dagger b_j \right) \left( b_i^\dagger b_j \right) \) is repulsive \([20]\). It is important to realize that this term involves nothing but the holon exchange interaction. Thus allowing the holon exchange channel for the quartic holon term (the second term in Eq. (3)), we obtain

\[ \frac{8t^2}{3J} \sum_{(i,j)} \left( b_i^\dagger b_j \right) \left( b_i^\dagger b_j \right) - \frac{J}{2} \sum_{(i,j)} \left( b_i^\dagger b_j b_i b_j + b_i^\dagger b_i b_j b_j \right) - \left( b_i^\dagger b_i b_j b_j \right) \]

(5)

We find from our numerical calculation of the Maxwell construction that the above holon exchange channel also affects phase separation, by effectively reducing the hopping (kinetic) energy. We find that with the neglect of the contribution of Eq. (3) the phase separation does not occur even at sufficiently low doping.

The effective holon attractive interaction term (when \( 0 < V < J/4 \) in the third term of Eq. (3)) \( - \sum_{(i,j)} \left( \frac{J}{4} - V \right) b_i^\dagger b_j b_j b_i \) can be decomposed into terms involving the direct, exchange, and pairing channels. The Hubbard-Stratonovich transformations and Bogoliubov-Valatin transformation in the momentum-space are made. As described in Ref. \([17]\), the mean field free energy at hole doping rate \( x \) is then

\[ F_{MF}(\chi, \Delta f, \Delta b) / N = 2J_{eff} |\chi|^2 + \frac{3J}{4} |\Delta f|^2 + (\frac{J}{2} - 2V) |\Delta b|^2 \]

\[ - 2T \sum_k \ln \left[ \cosh(\beta E_k^f / 2) \right] + T \sum_k \ln \left[ \sinh(\beta E_k^b / 2) \right] + (\frac{1}{2} + x) \mu_b - x \mu_f, \]  

(7)
Here $E_k^f = \sqrt{(\epsilon^f_k - \mu^f)^2 + \Delta^f_k^2}$ is the quasi-particle excitation energy for spinons and $E_k^b = \sqrt{(\epsilon^b_k - \mu^b)^2 - \Delta^b_k^2}$ for holons, where $\mu^f$ and $\mu^b$ are the effective chemical potentials of spinon and holon respectively and $\epsilon^f_k = -\frac{J^f}{\sqrt{\chi^f}} k \chi$, $\epsilon^b_k = -2t_{\text{eff}} k \chi$ with $\gamma_k \equiv \cos k_x + \cos k_y$. The effective Heisenberg coupling constant is $J_{\text{eff}} = \frac{3J^f n^f_0 + J^b n^b_0 - J^f n^f_0 - J^b n^b_0}{3J^f J^b n^f_0 n^b_0}$ and the effective holon hopping strength is $t_{\text{eff}} = \frac{2(n^f_0 + J^f - V)}{2n^f_0 + 3J^b n^b_0}$, where $\eta$ is the ratio of spinon and holon order parameter $\eta = \frac{(j^f_0 f^f_0)}{(n^f_0 b^f_0)}$.

From the minimization of the mean field free energy with respect to the scalar fields, $\chi$, $\Delta^f$, and $\Delta^b$, we determine the ground state energy density of the hole-doped system per site, $e_h(x) = \lim_{T \to 0} F_{\text{MF}}(\chi, \Delta^f, \Delta^b) / N$ as a function of hole density $x$. The critical hole density is actually found from the Maxwell construction by introducing $e(x) = (e_h(x) - e_H) / x$. In Fig. 1 we display the Maxwell’s construction for $J = 2.5t$ and $V = 0$. The inset is the Green function Monte Carlo calculation of the $t$-$J$ model by Hellberg and Manousakis [11]. Quantitative disagreement exists between our U(1) slave-boson functional integral approach and the Green function Monte Carlo calculation. However we find that there exists a minimum of $e(x)$ at the critical hole density of $x_c \sim 0.72$ which is close to the value of Hellberg and Manousakis [11], $x_c \sim 0.7$, below which phase separation occurs.

In Fig. 2 we display a predicted phase diagram in the plane of the unitless Heisenberg exchange coupling strength, $J/t$ and the electron density, $n = 1 - x$ for various values of NN hole-hole (holon-holon) repulsion energy $V$. The phase separation was predicted to occur for $J/t \lesssim 1$ and $J/t > 1$. This prediction is consistent with other numerical studies [11]. Green function Monte Carlo results [11] (solid line) up to the $28 \times 28$ square lattice and and the exact diagonalization result [3] (stars) with a $4 \times 4$ lattice are displayed for comparison with our results (solid circles for $V = 0$) with $100 \times 100$ lattice [21]. Despite some numerical differences, interestingly all of these methods yield nearly the same critical $J_c \sim 3.4t$, above which the hole-rich phase contains no spins, as shown in the Fig. 2. In the small $J/t$ limit, the phase separation is expected to occur as a result of relative increase in kinetic energy (compared to the Heisenberg interaction energy $J$) which promotes relatively easier hopping of holon (holes) from site to site, thus avoiding antiferromagnetic spinon (spin) frustrations to lower the energy of the system and creating a hole-rich region. On the other hand, in the large $J$ limit the phase separation occurs owing to the Heisenberg interaction coupling which promotes the antiferromagnetic order by inhibiting the occurrence of holes in the region of the antiferromagnetic phase [3].

![Fig. 1](image1.png)  
**FIG. 1.** Maxwell’s construction: $e(x)$ vs. $x$ for $J = 0.1t$, $V = 0$. The Green function Monte Carlo result [11] in the inset is denoted by HM.

![Fig. 2](image2.png)  
**FIG. 2.** Phase separation for the hole-doped systems of antiferromagnetically correlated electron in the plane of Heisenberg coupling strength, $J/t$ and the electron density, $n = 1 - x$. The solid line denoted by HM is the Monte Carlo prediction (Ref. [11]); and the stars denoted by EKL, the result of Emery et al (Ref. [5]); and the solid circles are our computed results for $V = 0$. The phase separation boundaries for $V = 0.125J$ (open circles) and $V = 0.25J$ (open triangles) are also displayed. The critical hole doping density $x_c$ is seen to decrease with the increase of $V$ in the region of large $J/t$. We now explore the effects of hole-hole (holon-holon) repulsive interaction $V$ on the phase separation boundary. The uniform phase is expected to be more favorable owing to the enhanced difficulty of hole pairing with the increase of $V$. The critical doping density in the physically interesting $J$ region, $J/t \lesssim 0.4$ is predicted to be relatively insensitive to the variation of $V$ compared to the high $J$ limit, as shown in Fig. 2. We observe that the critical hole doping density $x_c$ quickly decrease beyond the large $J$ region of $J/t > 0.4$ as the holon-holon (hole-hole) repulsion energy $V$ increases. For the case of the large $V$ limit ($V \sim 0.25J$), the uniform phase occurs with a small critical hole density, indicating the phase separation is not likely to occur. As shown in Fig. 2, we note the persistence of phase separation in the region of small $J$ and the propensity of gradual disappearance of phase
separation in the region of large $J/t$ at this high limit of the hole-hole repulsive interaction. Such persistence of phase separation at small $J/t$ despite the increase of $V$ is attributed to the effective increase of the kinetic energy of holons, to avoid the frustration of antiferromagnetic spinons \[5\].

In the present study we investigated the phase diagram involving phase separation based on the U(1) slave-boson functional integral approach to the $t$-$J$ model. We find that the phase separation occurs in the region of low hole doping for all possible values of Heisenberg coupling constant $J$, that is, whether $J/t < 1$ or $J/t \geq 1$ with an upper bound of $J/t$ (at $J \approx 4.2t$). This observation is consistent with other numerical studies of hole-doped two dimensional antiferromagnets.

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[21] Our numerical results are based on Eq. \[1\] at $T = 0$ limit which is expressed in momentum space. Numerical convergence was achieved for a $100 \times 100$ square lattice, which yielded a good convergence.