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Phase Separation Induced by Density-Dependent Hopping Terms

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We study phase separation in the $t - t' - J$ model in which the constraint of no double occupancy due to strong electron correlations leads to effective narrowing of the band width. Using a mean-field approximation, we calculate the compressibility in the normal state and show that the phase separation can be induced by the variation of the band width.

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Spontaneous lattice symmetry breaking in electron density is widely observed in strongly correlated electron systems, e.g., high-T_c cuprate superconductors in which charge ordered states occur in a wide region of the temperature (T)- doping rate (δ) phase diagram.[1] In theoretical models without long-range Coulomb interactions such as the Hubbard and $t-J$ models, phase separation (PS) is known to appear as a typical inhomogeneous electron density state.[2–20] Especially in Refs. 12 and 13, the location of the PS region in the phase diagram was intensively investigated by applying the $1/N$ expansion method to the $t-J$ model.

In the $t-J$ model, double occupancy of a single site is prohibited due to the strong electron correlation. When this condition is treated using slave-boson mean-field (SBMF) or Gutzwiller approximations, transfer integrals are multiplied by the doping rate δ (< 1) and thus reduced. These density-dependent transfer integrals lead to the narrowing of the band width. Recently, it is demonstrated that density-dependent hopping terms exist in the effective single-band Hamiltonian for the cuprates that is derived from the three band model using the density matrix renormalization group method.[21] This suggests that the hopping process in strongly correlated electron systems may depend on the site occupancy in general, and it may lead to spontaneous lattice symmetry breaking of electron density, namely, phase separation and charge order.

In this short note, we study the effect of density-dependent hopping terms on the phase separation. We employ the $t-t'-J$ model ($t-J$ model with extended transfer integrals) and treat it within the SBMF approximation as a test case to explore this problem. We investigate the compressibility in the normal metallic (uniform RVB) state but not in ordered states, in order to focus on the band narrowing effect on the phase separation.

We treat the $t-t'-J$ model on a square lattice with the Hamiltonian,

$$H = -\sum_{j,\ell,\sigma} t_{j\ell}\tilde{c}^{\dagger}_{j\sigma}\tilde{c}_{\ell\sigma} + J\sum_{\langle j,\ell\rangle}\mathbf{S}_j\cdot\mathbf{S}_\ell, \tag{1}$$

where the transfer integrals $t_{j\ell}$ are finite for the first- (t) and second- (t') nearest-neighbor bonds, or zero otherwise. J is the antiferromagnetic superexchange interaction, and $\langle j,\ell\rangle$ denotes nearest-neighbor bonds. $\tilde{c}_{j\sigma}$ is the operator for the electrons in Fock space without double occupancy. We treat this condition using the SBMF theory assuming the Bose condensatoin of holons,[20,22] and write spinon operator as $f_{j\sigma}$.

In order to study the phase separation in the normal state, we decouple this Hamiltonian by employing only $\chi_f = \sum_\sigma\langle f^{\dagger}_{j\sigma}f_{j+\eta\sigma}\rangle$ ($\eta = \pm\hat{x},\pm\hat{y}$) as an order parameter (bond order parameter). Selfconsistency equations are obtained by minimizing the free energy and given as,

$$n = \frac{2}{N}\sum_k f(\xi_k), \;\; \chi_f = \frac{1}{N}\sum_k \gamma_k f(\xi_k) \tag{2}$$

where n $(= 1 - \delta)$ and N are the electron density and the total number of lattice sites, respectively, $\gamma_k = \cos k_x + \cos k_y$ and $\xi_k = -2(t\delta + \frac{3J}{8}\chi_f)\,\gamma_k - 4t'\delta\cos k_x \cos k_y - \mu$ with μ being the chemical potential. $f(\xi_k)$ is the Fermi distribution function.

By taking derivatives of Eq.(2) with respect to μ, we obtain simultaneous equations for the compressibility, $\partial n/\partial\mu$, and $\partial\chi_f/\partial\mu$,

$$\hat{A}\begin{pmatrix} \dfrac{\partial n}{\partial \mu} \\ \dfrac{\partial \chi_f}{\partial \mu} \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \tag{3}$$

where $\hat{A}$ is a 2×2 matrix with $A_{11} = 1 - \frac{2}{N}\sum_k \Gamma_k f'(\xi_k)$, $A_{12} = \frac{3J}{2N}\sum_k \gamma_k f'(\xi_k)$, $A_{21} = -\frac{1}{N}\sum_k \gamma_k\Gamma_k f'(\xi_k)$, and $A_{22} = 1 + \frac{3J}{4N}\sum_k \gamma_k^2 f'(\xi_k)$. Here $\Gamma_k = 2t\gamma_k + 4t'\cos k_x\cos k_y$, $c_1 = -\frac{2}{N}\sum_k f'(\xi_k)$, and $c_2 = -\frac{1}{N}\sum_k \gamma_k f'(\xi_k)$. By solving Eq.(3), we get $\partial n/\partial\mu = (A_{22}c_1 - A_{12}c_2)/D$ and $\partial\chi_f/\partial\mu = -(A_{21}c_1 - A_{11}c_2)/D$ with $D = A_{11}A_{22} - A_{12}A_{21}$.

For comparison, we also calculate the compressibility by dropping the derivatives of δ's in ξ_k. Namely, we treat them constants independent of μ. It simply amounts to set $\Gamma_k = 0$, and so $A_{11} = 1$ and $A_{21} = 0$. We denote the compressibility in this case as $(\partial n/\partial\mu)_0$.

In Fig.1 we show the results for the compressibility, $\partial n/\partial\mu$, for several choices of T. We take the parameters $J = 1$, $t/J = 2.5$, $t'/t = \pm 0.3$. The t' term is introduced to change the Fermi surface and to examine its effect. In the case of $t'/t = 0.3$, the compressibility is positive for $\delta \gtrsim 0.1$, i.e., the region relatively away from half filling, and the homogeneous state is stable here. The compressibility diverges at the transition point $\delta \sim 0.1$, and becomes negative near half-filling. Thus the homogeneous state is not stable in this region and the phase separation occurs. In numerical calculations, if we take δ as an input parameter a spurious solution may be obtained, but the compressibility diverges (or becomes negative). When the resultant μ is taken as an input parameter, we cannot obtain the original value of δ, since multiple values of δ corresponds to a single value of μ. In the case of $t'/t = -0.3$, the compressibility is always finite and positive in the region studied and so the homogeneous state is stable. This means that the occurence of phase separation depends on the band structure, in other words, the shape of the Fermi surface. In Ref.13, the PS region also appears for negative t' cases. The reason for the difference is that the Hamiltonian in Ref.13 includes the term $-J\sum_{\langle j,l\rangle} n_j n_l/4$, which is an attractive interaction between nearest-neighbor sites, and it will help to induce (enhance) the PS state. (Actually if we include this term in H, phase separated states occur for $t'/t = -0.3$ near $\delta = 0$.)

In Fig.2 we present the results for $(\partial n/\partial\mu)_0$, which does not take into account the variation of the band width with μ. It is seen that $(\partial n/\partial\mu)_0$ is always finite and positive for both $t'/t = 0.3$ and $t'/t = -0.3$, in contrast to the case of $\partial n/\partial\mu$. This indicates that the variation of the band width is responsible for the appearance of the phase separation.

Results for $\partial\chi_f/\partial\mu$ are shown in Fig.3 for both $t'/t = 0.3$ and $t'/t = -0.3$. The former diverges at the phase transition point, while the latter is an analytic function, as expected from the behavior of $\partial n/\partial\mu$.

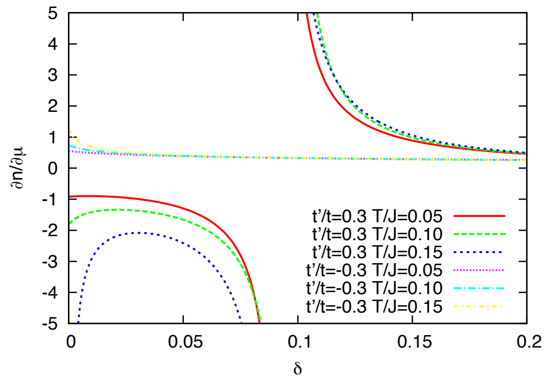

Fig. 1. (Color online) Compressibility $\partial n/\partial\mu$ for $t'/t = 0.3$ and $t'/t = -0.3$ with temperatures $T/J = 0.05$, $T/J = 0.10$, and $T/J = 0.15$.

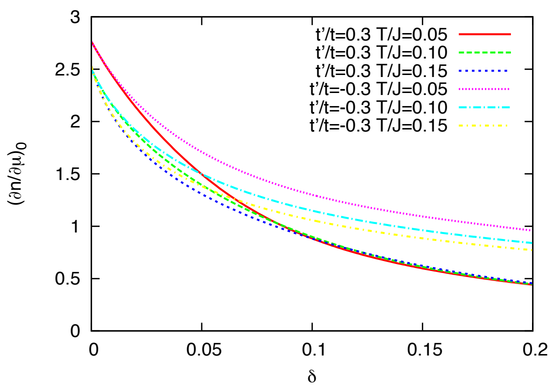

Fig. 2. (Color online) Compressibility $(\partial n/\partial\mu)_0$ for $t'/t = 0.3$ and $t'/t = -0.3$ with temperatures $T/J = 0.05$, $T/J = 0.10$, and $T/J = 0.15$.

In summary, we have calculated the compressibility in the normal state of the $t - t' - J$ model. It is found that the variation of the band width due to strong electron correlations can

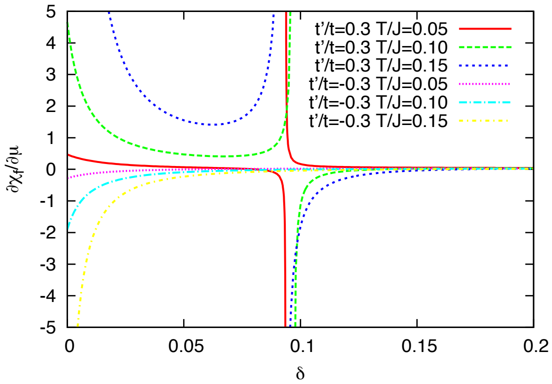

Fig. 3. (Color online) $\partial\chi_f/\partial\mu$ for $t'/t = 0.3$ and $t'/t = -0.3$ with temperatures $T/J = 0.05$, $T/J = 0.10$, and $T/J = 0.15$.

induce phase separation, but its occurence depends on the band structure, in other words, the shape of the Fermi surface.

The density-dependent hopping terms may induce charge ordered states as well as phase separation, and it will be intriguing to explore this possibility. In these studies, the inclusion of the long-range Coulomb interaction may be necessary, since it would suppress the phase separated states strongly compared with other states, and thus affect the competition among the candidate states.

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