Phase separation and *d*-wave superconductivity in a two-dimensional extended Hubbard model with nearest-neighbor attractive interaction

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Inhomogeneities on various length scales suggesting phase separation seem to be a generic feature of hole-doped high-temperature superconducting cuprates. Also firmly established is the *d*-wave symmetry of the superconducting state. The interplay of superconductivity and phase separation has been noted in previous mean-field studies of correlated electron models. To further explore this issue in a more rigorous approach we have conducted quantum Monte Carlo calculations of a two-dimensional Hubbard model with nearest-neighbor attractive interaction. For a vanishing on-site repulsion, the result agrees with that of Micnas, Ranninger, and Robaszkiewicz [Phys. Rev. B **39**, 11 653 (1989)], and indicates that for a given strength of the attractive interaction, homogeneous *d*-wave superconducting phase can exist only above a critical doping concentration, below which phase separation occurs. A finite on-site repulsion modifies the phase separation behavior. A stronger *d*-wave pairing correlation is seen in the inhomogeneous phase compared to the homogeneous phase.

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An impressive amount of experimental work on hole-doped high-temperature superconducting cuprates has revealed an almost ubiquitous presence of inhomogeneities on various length scales. For example Pan *et al.*[1] have detected a wide distribution of *d*-wave superconducting gaps on the surface of $Bi_2Sr_2CaCu_2O_{8+x}$ on the nanometer scale. A recent scanning superconducting quantum interference device microscopy study by Iguchi *et al.*[2] has reported the existence of micrometer-sized diamagnetic islands well above T_c in $La_{2-x}Sr_xCuO_4$. On top of those is the well-known phase separation found to occur in oxygen-doped $La_2CuO_{4+\delta}$ (Ref. 3) and related systems.[4] All those notorious deviations from a homogeneous state demand a serious theoretical answer.

Indeed, there has also been much theoretical effort to look for models which exhibit phase separation[5] or related behaviors. The repulsive Hubbard model (or its equivalent models) has been extensively scrutinized towards this end. However, there are indications that this type of model supports neither superconductivity[6,7] nor phase separation.[8,9] A model which does seem to support both is the extended Hubbard model with an attractive nearest-neighbor interaction V (the t-U-V model[10]). Lin and Hirsch[11] studied the one-dimensional version of this model in the half-filled sector and found that a first-order condensation transition occurs at a critical value of V which is a function of the on-site repulsion U. Within mean-field and random-phase approximations Micnas, Ranninger and Robaszkiewicz[12] (MRR) examined the stability of *d*-wave superconductivity with respect to phase separation in the two-dimensional t-U-V model. For each band filling, they found that the superconducting state is unstable above a critical strength of V. The proximity of phase separation to superconductivity in the parameter space of models of correlated electrons was emphasized by Dagotto *et al.*,[13] who also mentioned an attempt to carry out a more rigorous quantum Monte Carlo study of the two-dimensional t-U-V model. Some result from such a study was reported by Nazarenko, Moreo and Dagotto.[14] Their calculations were quite limited and led the authors to conclude that the t-U-V model is not a useful model for *d*-wave superconductivity. Recently, Shaw and Su[15] did a quantum Monte Carlo study of a simplified version of the attractive t-V model and found both phase separation and *d*-wave superconductivity. The current paper describes the results of more extensive quantum Monte Carlo calculation of the two-dimensional t-U-V model.

The t-U-V model is defined as

$$H=-t\sum_{\langle ij\rangle\sigma}[c_{i\sigma}^{\dagger}c_{j\sigma}+\mathrm{H.c.}]+U\sum_{i}\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)+V\sum_{\langle ij\rangle}(n_i-1)(n_j-1)-\mu\sum_{i}n_i, \tag{1}$$

where $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ is a density operator of the conduction electrons, $\langle ij\rangle$ is a nearest neighbor pair. For negative V this model has been widely used to model the *d*-wave phenomenologies of the cuprates under various mean-field approximations. Huang *et al.*[16] have briefly examined the superconducting properties of this model using the constrained-path Monte Carlo technique. For studying the phase separation, the determinantal quantum Monte Carlo[17] is particularly suitable as it is a grand canonical formalism. This is the methodology we adopt for this work. For convenience, we set $t=1$ in what follows.

To present our results, we focus on the two equal-time correlation functions, the *s*-wave pair field correlation function

$$P_s=\langle\Delta\Delta^{\dagger}\rangle, \tag{2}$$

with

$$\Delta^{\dagger}=\frac{1}{\sqrt{N}}\sum_{\mathbf{l}}c_{\mathbf{l}\uparrow}^{\dagger}c_{\mathbf{l}\downarrow}^{\dagger}, \tag{3}$$

and the *d*-wave counterpart

$$P_d=\langle\Delta_d\Delta_d^{\dagger}\rangle, \tag{4}$$

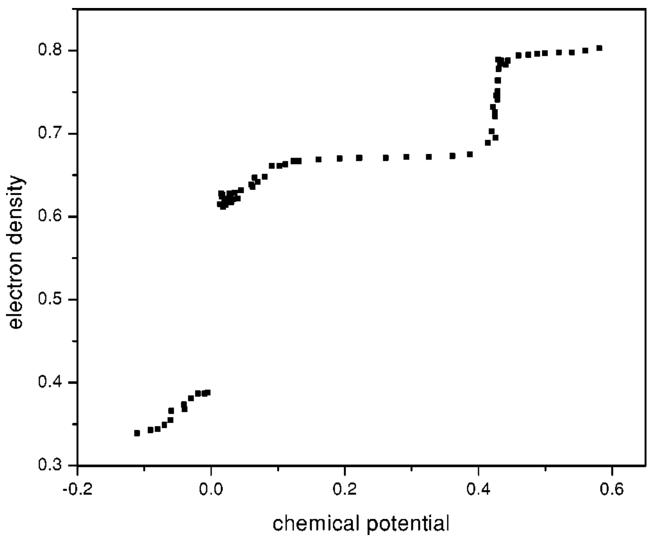

FIG. 1. Average electron density per spin as a function of chemical potential. The calculations were done on an 8×8 lattice at inverse temperature $\beta=15$ and for $U=0$ and $V=-0.5$.

with

$$\Delta_d^\dagger=\frac{1}{4\sqrt{N}}\sum_{\mathbf{l},\delta} c_{\mathbf{l}\uparrow}^\dagger c_{\mathbf{l}+\delta\downarrow}^\dagger(-1)^\delta. \tag{5}$$

Based on what is learnt from the repulsive Hubbard model, the long-range part of the pair-field correlation is a better indicator[6,7] than the fully intergrated one. Therefore we exclude near neighbors in the double summation (over $\mathbf{l}$ and $\mathbf{l}'$) in Eqs. (2) and (4). For the 8×8 lattice results to be described, neighbors ($\mathbf{l}$ and $\mathbf{l}'$) with distance less than three lattice spacings are excluded. The determinantal Monte Carlo algorithm is quite straightforward to implement for this model, the only problem is the sign problem. In the lowest temperature T we have reached $\beta=1/T=15$, the average sign is about 0.1 in the worst case.

To isolate the connection between superconductivity and phase separation from antiferromagnetism, we first turn off the U term. Fig. 1 is a plot of the average electron density (per spin per site) as a function of the chemical potential. The inverse temperature is $\beta=15$ and the attractive interaction is $V=-0.5$. There is a clear discontinuity and a density gap exists near $\mu=0$. The size of this gap increases rapidly with the magnitude of V. For $V=-0.75$, the gap size is 0.75. For $V=-1$, the size has almost reached its maximum value 1. The gap size in Fig. 1 is about 0.23. The corresponding numbers for the 6×6 and 10×10 lattices are 0.28 and 0.20, respectively. A simple linear extrapolation (Fig. 2) of the gap size versus the inverse linear dimension of the lattice yields a limit 0.08 for the infinite lattice, in good agreement with the value 0.06 obtained by MRR.[12] The existence of the density gap[18] is a clear demonstration of phase separation. A homogeneous phase can exist only for a certain range of density. At half-filling, for example, the system can exist only as a phase-separated state consisting of electron-rich and other hole-rich components.[19]

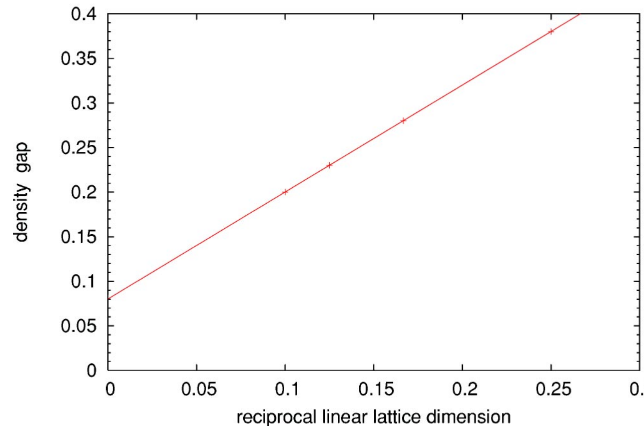

FIG. 2. (Color online) Plot of the density gap vs the reciprocal linear lattice dimension.

To examine the superconducting properties of the allowed homogeneous phases, we show the long-range part of the d-wave pair-field correlation function as a function of band filling in Fig. 3. Compared with the correlation function of the noninteracting system there is a significant enhancement. The negative V also enhances the s-wave correlation to a less extent, but as will be seen shortly this enhancement is easily counteracted by the on-site repulsion U. Together Figs. 1 and 3 imply that a nearest-neighbor attractive interaction underlies both d-wave superconductivity and phase separation.

For $V=0$ the repulsive Hubbard model has been extensively studied, and it is understood that antiferromagetic correlations dominate near half-filling. Therefore we would expect a gradual filling up of the density gap as a finite U is restored. With that in mind, we have carried out another calculation for $U=-V=0.5$. Because of the sign problem, we have to raise the temperature to $\beta=7$. As seen from Fig. 4,

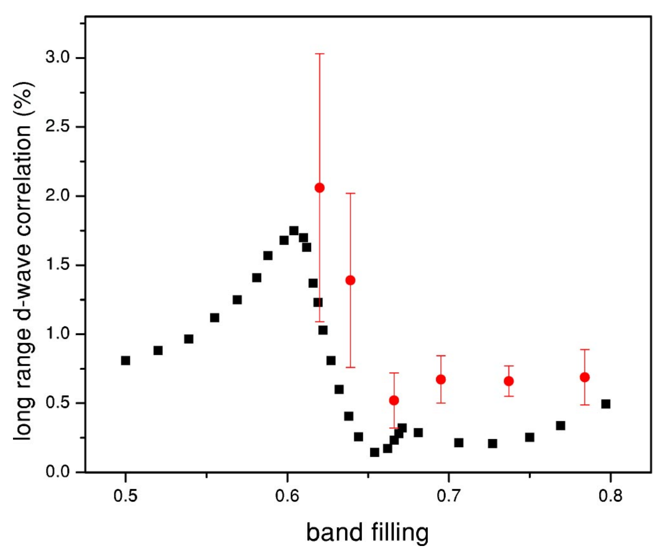

FIG. 3. (Color online) Long-range d-wave correlation P_d (in units of 0.01) as a function of band filling for the same lattice and temperature as in Fig. 1. The circles are for $V=-0.5$ and the squares are for $V=0$. U is set to zero in both cases.

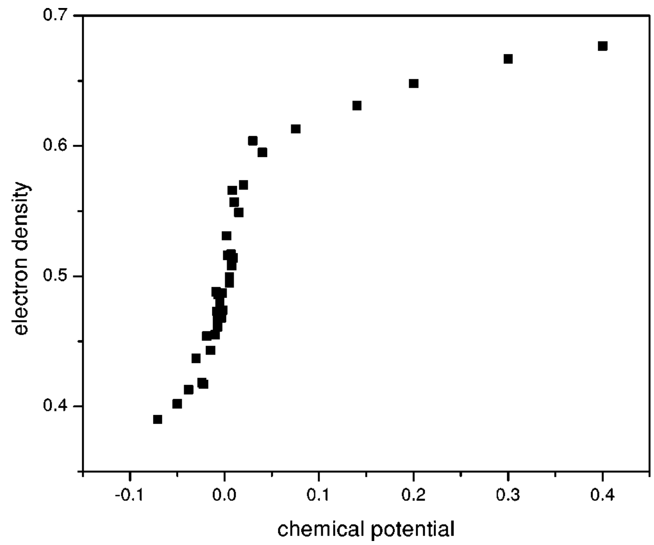

FIG. 4. Average electron density per spin as a function of chemical potential on an 8×8 lattice at inverse temperature $\beta=7$ and for $U=-V=0.5$.

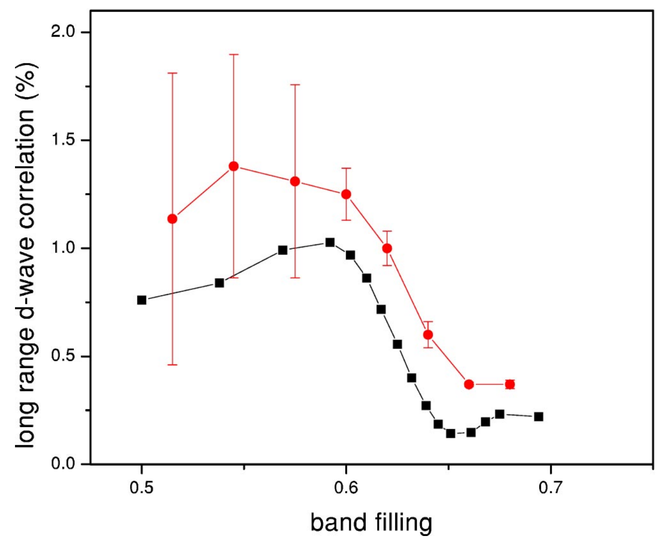

FIG. 6. (Color online) Long-range d-wave correlation P_d (in units of 0.01) as a function of band filling. The circles are for $U=-V=0.5$ and the squares are for $U=V=0$. The lattice size and temperature are the same as in Fig. 4.

the density gap near half-filling is indeed filled. The slope of the n vs μ curve remains steep near $\mu=0$, suggesting that the system is still very close to a phase separation. To throw more light on this issue, we examine the distribution of electron density of several simulation runs corresponding to an average density of 0.5, 0.55, 0.59, and 0.61 in Fig. 5. One sees a wide distribution covering nearly the entire original density gap for all the average densities below 0.6. As the average density approaches the original gap edges, the distribution narrows down, as it should for a homogeneous phase. We take the wide dispersion of the density distributions in Fig. 5 as evidence of phase separation for a finite

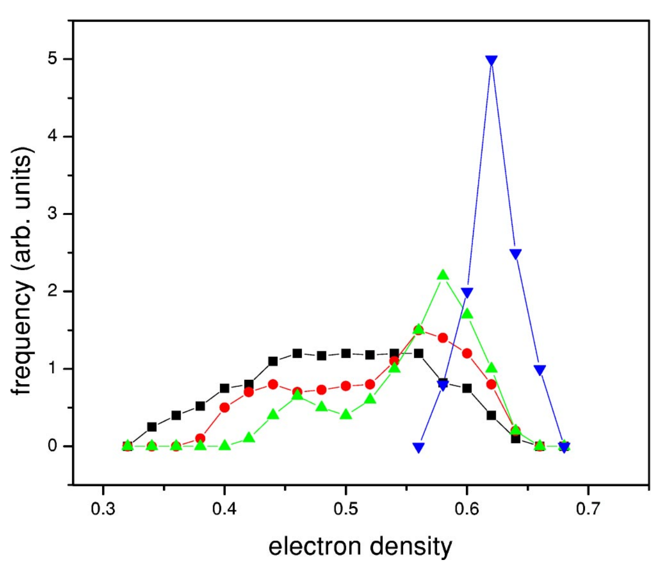

FIG. 5. (Color online) Distribution of the electron density in a typical simulation run corresponding to an average electron density of 0.5 (square), 0.55 (circle), 0.59 (triangle), and 0.61 (inverted triangle), respectively. The lattice size, temperature, U, and V are the same as in Fig. 4.

on-site repulsion. As for the superconducting correlation functions, the d wave is still enhanced (Fig. 6) with respect to the noninteracting value over a wide range of density, but the s wave is suppressed. For a large enough U, eventually the d-wave superconductivity is suppressed[16] too.

Another notable feature of Fig. 6 is that the d-wave correlation actually peaks inside the gap rather than at the original density gap edge. In other words, certain phase-separated states seem to have a stronger superconducting correlation than the homogeneous phase. In addition, the large fluctuations (the error bars) in the superconducting correlation may be intrinsic and reflect the inhomogeneous superconductivity. The doping dependence of the d-wave correlation is similar to what is observed in the cuprates if one identifies the overdoped region with the homogeneous states, and the underdoped region with the inhomogeneous states.

Upon further increase of U for a fixed V, the sign problem worsens. It becomes more difficult to lower the temperature enough to ascertain whether a phase separation occurs.

To further relate the results of this paper to high-temperature superconductivity, a comment is in order. The t-U-V model possesses an electron-hole symmetry that is absent in the cuprates. In addition, the antiferromagnetic state near half-filling $n_1=0.5$ is stabilized by larger values of U. Thus we speculate that in the hole-doped cuprates, the two phases involved in the phase separation are the antiferromagnetic phase $n_1=0.5$ and a hole-rich terminal phase $n_2<n_1$.

In conclusion, we believe that the t-U-V model should be taken more seriously as a model for d-wave superconductivity. The nearest-neighbor attractive interaction should be regarded as something more than a mathematical device to generate d-wave superconductivity. If it is really physical, then one ought to think more critically about where it comes from.[20] Exciton mediated interaction is a natural possibility and the idea is currently being explored.[21] Finally we mention that the simultaneous absence of *d*-wave superconductivity and phase separation tendency in the electron-doped cuprates[22] is consistent with our model calculations.

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