

# Mott correlated states in the underdoped two-dimensional Hubbard model: Variational Monte Carlo versus a dynamical cluster approximation

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We investigate the properties of the frustrated underdoped Hubbard model on the square lattice using two complementary approaches, i.e., the dynamical cluster extension of the dynamical mean-field theory and the variational Monte Carlo simulations of Gutzwiller-Jastrow wave functions with backflow corrections. We compare and discuss data for the energy and the double occupancies, as obtained from both approaches. At small dopings, we observe a rapid crossover from a weakly correlated metal at low interaction strength  $U$  to a non-Fermi-liquid correlated state with strong local spin correlations. Furthermore, we investigate the stability of the correlated state against phase separation. We observe phase separation only for large values of  $U$  or very large frustration. No phase separation is present for the parameter range relevant for the cuprates.

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## I. INTRODUCTION

The Hubbard model on the square lattice is a minimal model for describing electronic correlation. This model has played a central role in the study of high- $T_C$  superconductivity, since it is believed to capture the essential physics of the copper-oxygen planes in cuprate materials. Furthermore, the properties of the Hubbard model in the underdoped regime, i.e., in the proximity of the Mott-insulating state at half filling, is a stimulating research area due to the challenge of describing the physics of the correlated pseudogap state and its non-Fermi-liquid behavior. Significant achievements in this field have been made, for instance, by the cluster extensions of dynamical mean-field theory,<sup>1-7</sup> by means of a phenomenological theory<sup>8</sup> and the Gutzwiller approximation,<sup>9</sup> as well as on the basis of increasingly accurate variational wave functions.<sup>10,11</sup>

Recently, it has been proposed that the pseudogap and the superconducting phases present at finite doping<sup>12-14</sup> and for onsite  $U$  values corresponding to a Mott-insulating state at half filling can be continuously connected to a pseudogap and a superconducting phase at half filling for  $U$  values lower than the critical  $U_c$  corresponding to the Mott-Hubbard metal-insulator transition (MIT). This proposal contrasts with Anderson's concept of superconductivity as a state emerging out of a resonant valence bond (RVB) state,<sup>15</sup> which is a prototypical Mott-insulating state at half filling in the absence of magnetic order.

Another interesting feature of a correlated electron state in the underdoped regime is the tendency of the system to phase separate into an undoped state with strong antiferromagnetic correlations and a hole-doped region. Indeed, if the Hubbard model would be unstable to phase separation, its validity as a model to properly describe the development of superconductivity could be questioned. Phase separation occurs when the stability condition  $\partial^2 E(n)/\partial n^2 > 0$  is violated, i.e., when the ground-state energy  $E(n)$ , as a function of electronic density  $n$ , is no longer convex. As introduced by Emery *et al.*,<sup>16</sup> phase separation can be studied by looking at the hole energy  $E_\delta(\delta)$ , defined as

$$E_\delta(\delta) = \frac{E(\delta) - E(0)}{\delta}, \quad (1)$$

where  $\delta = 1 - n$  is the hole density. If the hole energy has a minimum at a critical doping  $\delta_c$ , then the system is unstable to phase separation for  $\delta < \delta_c$ . A difficulty when using the Emery criterion (1) is its strong dependence on the accuracy in the estimate of the ground-state energy, as discussed in Ref. 17. In particular, less accurate ground-state energies tend to overestimate the critical  $\delta_c$  below which the system exhibits phase separation. This is a consequence of the fact that good estimates for the energy of low-doping states are hard to obtain because of the strong local correlations. Different approaches have led in the past to contradictory results for the Hubbard model in the parameter range relevant for hole-doped cuprates, ranging from an absence of phase separation to a range of estimates for phase separation up to 10% doping.<sup>18-24</sup> For the  $t - J$  model,<sup>25-28</sup> i.e., for the large- $U$  limit of the Hubbard model, phase separation is present at all dopings for large values of  $J$ , but the possible occurrence of phase separation close to half filling for small values of  $J$  has been a long-standing debate.<sup>26-28</sup>

In this work, we make use of variational Monte Carlo (VMC) simulations, including backflow correlations,<sup>29</sup> and of the dynamical cluster approximation (DCA)<sup>30,31</sup> to address the properties of the Hubbard model on the square lattice with nearest- and next-nearest-neighbor hoppings in the underdoped regime, both at zero and finite temperature. As already pointed out in Ref. 11, we distinguish a weakly correlated metal at small  $U$  (i.e., continuously connected to a half-filled metallic regime) and a strongly correlated state at intermediate to large  $U$  (i.e., when the half-filled case is insulating). We find significant differences between the two regimes in the static and in the dynamical spin correlations as well as in the low-energy part of the self-energy. The above observations obtained from two complementary approaches, VMC and DCA, and the violation of the Luttinger sum rule for the strongly correlated state reported in a previous study<sup>11</sup> hint to a non-Fermi-liquid nature of the strongly correlated state. The two states are separated by a crossover line at the critical interaction  $U_c$ , which may evolve into a first-order transition<sup>6</sup> when doping is vanishing.

Moreover, we investigate the occurrence of phase separation in the underdoped Hubbard model. We find no tendency

to phase separation when the Coulomb repulsion  $U$  is slightly above the critical  $U_c$ , regardless of the ratio  $t'/t$  between next-nearest- and nearest-neighbor hoppings,  $t'$  and  $t$ , respectively. Our results therefore indicate that for intermediate values of the Coulomb repulsion ( $U/t \sim 6-8$ ), the Hubbard model is stable against phase separation, irrespective of the value of  $t'/t$ . The actual value of  $t'/t$  is sensitive to the details of the high- $T_c$  cuprate compound investigated and can be calculated, for example, in density functional theory, leading to  $t'/t \simeq [-0.1, -0.4]$ . A larger degree of frustration has been shown to correlate, in general, with higher critical temperatures.<sup>32</sup>

If we increase the electron repulsion  $U$  at constant  $t'/t$ , then the system is, in contrast, found to be unstable towards phase separation. However, since increasing the variational accuracy tends to suppress phase separation, we cannot exclude that an even more accurate approach could eliminate or significantly reduce the tendency to phase separate also for larger values of the Coulomb repulsion.

The paper is organized as follows: in Sec. II, we introduce the Hamiltonian and describe the VMC and the DCA approaches. In Sec. III, we compare ground-state energy and the density of double occupancies within the two methods. In Sec. IV, we discuss the non-Fermi-liquid properties of the underdoped region at  $U > U_c$ , in contrast with the weakly correlated metal at  $U < U_c$ . In Sec. V, the occurrence of phase separation is discussed, and, finally, we present our conclusions in Sec. VI.

## II. MODEL AND METHODS

We consider the frustrated Hubbard model with extended hopping on a two-dimensional (2D) square lattice,

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - t' \sum_{\langle\langle ij \rangle\rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (2)$$

where  $c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) denotes the electron creation (annihilation) operator of one electron on site  $i$  with spin  $\sigma = \uparrow, \downarrow$ ;  $\langle ij \rangle$  and  $\langle\langle ij \rangle\rangle$  indicate nearest- and next-nearest-neighbor sites, respectively;  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$  is the electron density;  $t$  and  $t'$  are the nearest- and next-nearest-neighbor hopping amplitudes, respectively; and  $U$  is the on-site Coulomb repulsion.

### A. Variational Monte Carlo

Variational Monte Carlo (VMC) simulations allow one to perform nonperturbative calculations at zero temperature for one- and two-dimensional correlated and frustrated systems. VMC simulations are based on numerically sampling expectation values over a variational estimate of the ground-state wave function. Here we will use a powerful variational *ansatz* for frustrated electron systems, which has been strictly tested by extensive comparisons to analytical and numerical exact limiting cases. Our variational *ansatz* has been tested, in particular, against Bethe *ansatz* predictions for the Luttinger liquid exponents in one dimension,<sup>33</sup> with respect to Lanczos results in terms of wave-function overlap for a two-dimensional 18-site cluster,<sup>34</sup> and with respect to the results of density-matrix renormalization group studies in terms of the ground-state energy for the 1D  $J_1$ - $J_2$  model.<sup>29</sup>

The variational *ansatz* consists of three components. In a first step, we construct uncorrelated nonmagnetic wave functions given by the ground state  $|\text{BCS}\rangle$  of a superconducting Bardeen-Cooper-Schrieffer (BCS) Hamiltonian:<sup>35-37</sup>

$$\mathcal{H}_{\text{BCS}} = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_k \Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \text{H.c.}, \quad (3)$$

where both the free-band dispersion  $\xi_k$  and the pairing amplitudes  $\Delta_k$  are variational functions. We use the parametrization

$$\xi_k = -2\tilde{t}(\cos k_x + \cos k_y) - 4\tilde{t}' \cos k_x \cos k_y - \mu, \quad (4)$$

$$\Delta_k = 2\Delta_{\text{BCS}}(\cos k_x - \cos k_y), \quad (5)$$

where the effective hopping amplitude  $\tilde{t}$ , the effective chemical potential  $\mu$ , and the local pairing field  $\Delta_{\text{BCS}}$  are variational parameters to be optimized in order to minimize the variational energy. The parameter  $\tilde{t}$  is kept fixed to set the energy scale. We point out that large electronic correlations, as in proximity of a Mott insulator, lead to a strong renormalization of  $\tilde{t}$  with respect to the bare Hamiltonian value  $t'$ ; see Ref. 11.

The correlated state  $|\Psi_{\text{BCS}}\rangle$ , without backflow terms, is then given by  $|\Psi_{\text{BCS}}\rangle = \mathcal{J}|\text{BCS}\rangle$ , where  $\mathcal{J} = \exp(-1/2 \sum_{ij} v_{ij} n_i n_j)$  is a density-density Jastrow factor (including the on-site Gutzwiller term  $v_{ii}$ ), with the  $v_{ij}$ 's being optimized for every independent distance  $|i - j|$ . Notably, within this kind of wave function, it is possible to obtain a pure (i.e., nonmagnetic) Mott insulator for a sufficiently singular Jastrow factor  $v_q \sim 1/q^2$  (where  $v_q$  is the Fourier transform of  $v_{ij}$ ), while a superconducting (metallic) state is found whenever  $v_q \sim 1/q$  and  $\Delta_{\text{BCS}} > 0$  ( $\Delta_{\text{BCS}} = 0$ ).<sup>33</sup>

A size-consistent and efficient way to further improve the correlated state  $|\Psi_{\text{BCS}}\rangle$  for large on-site interactions is based on backflow correlations. In this approach, each orbital that defines the unprojected state  $|\text{BCS}\rangle$  is taken to depend upon the many-body configuration in order to incorporate virtual hopping processes;<sup>29</sup> in particular the recombination of neighboring charge fluctuations is favored. This is a substantial improvement with respect to Jastrow factors, where electron-electron correlation is included only via a multiplicative term. All results presented here are obtained by fully incorporating the backflow corrections and optimizing individually<sup>38</sup> every variational parameter in  $\xi_k$  and  $\Delta_k$ , in the Jastrow factor  $\mathcal{J}$  as well as for the backflow corrections. Calculations are performed on 45° tilted clusters with  $L = 162$  lattice sites and periodic boundary conditions.

### B. Dynamical cluster approximation

DCA is the cluster extension of single-site dynamical mean-field theory (DMFT),<sup>39</sup> which includes, to a certain degree, momentum dependencies. Since the hopping matrix for sites within the considered cluster and for sites on different clusters is the same, in contrast to the cellular DMFT approach,<sup>40</sup> the DCA self-consistent equation can be written in momentum space with the assumption that the self-energy is constant in the Brillouin-zone sectors that are considered. The DCA self-consistency equation is given as

$$\bar{G}_\sigma(\mathbf{K}, i\omega_n) = \frac{1}{N} \sum_{\mathbf{K}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{K}+\mathbf{K}} - \Sigma_\sigma(\mathbf{K}, i\omega_n)}, \quad (6)$$

where  $N$  is the number of  $k$  points in each Brillouin-zone sector (compare Fig. 3),  $\mu$  is the chemical potential,  $\mathbf{K}$  is the cluster momentum,  $\epsilon_{\mathbf{k}+\mathbf{K}}$  is the dispersion relation,  $\omega_n$  are the fermionic Matsubara frequencies, and where the summation over  $\mathbf{K}$  is performed in each Brillouin-zone sector. In our calculations, we employed the DCA cluster with  $N_c = 4$ , where  $\mathbf{K} = (0,0), (0,\pi), (\pi,0)$ , and  $(\pi,\pi)$ . The converged self-energy  $\Sigma_\sigma(\mathbf{K}, i\omega_n)$  is evaluated by means of Eq. (6) and the Dyson equation. We employ the interaction expansion continuous-time quantum Monte Carlo approach as an impurity solver.<sup>41,42</sup> All calculations presented here are for a temperature  $T/t = 0.05$  and we perform more than  $10^7$  quantum Monte Carlo (QMC) samplings for the impurity Green's function  $G(i\omega_n)$ , in order to keep the QMC statistical errors smaller than  $5 \times 10^{-3}$  for the first Matsubara frequency. As the Matsubara frequencies increase, the error bar decreases.

### III. ENERGY AND DOUBLE OCCUPANCIES

In Fig. 1, we compare the average number of double occupancies per site  $D = \langle n_{i,\uparrow}n_{i,\downarrow} \rangle$  and the energy, for  $U/t = 7.0$  and  $t'/t = -0.4t$  as a function of the electron density  $n$ , as obtained from VMC and DCA simulations. For the DCA calculations, the energy is calculated by

$$E = \frac{T}{N} \sum_{n,k,\sigma} [\epsilon_k \bar{G}_\sigma(\mathbf{k}, i\omega_n)] e^{i\omega_n, 0^+} + UD, \quad (7)$$

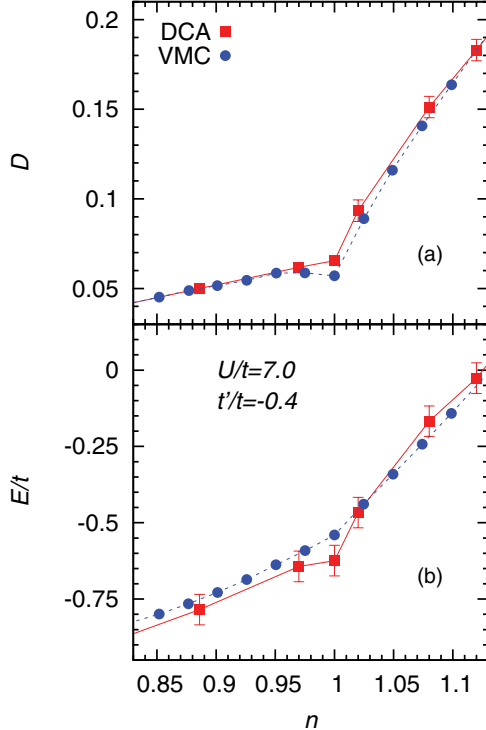


FIG. 1. (Color online) (a) Double occupancy  $D$  and (b) energy as a function of electronic density  $n$  for  $U/t = 7.0$  and  $t'/t = -0.4t$ . Results are obtained using a VMC approach on an  $L = 162$  lattice size (blue circles) and within DCA by means of a  $2 \times 2$  plaquette in  $k$  space for a temperature  $T/t = 0.05$  (red squares). Errors in VMC are smaller than the symbol size. Lines are just guides to the eye.

where the index  $\mathbf{k}$  runs over the first Brillouin zone and we considered the asymptotic behavior of the self-energy in the limit of large Matsubara frequencies  $i\omega_n$ :  $\Sigma_\sigma(\mathbf{K}, i\omega_n) \sim U^2 n_\sigma (1 - n_\sigma) / i\omega_n$ . The error  $\Delta_n$  of the self-energy  $\Sigma(i\omega_n)$  is calculated by

$$\Delta_n = \frac{2\xi}{G(i\omega_n)^2}, \quad (8)$$

where  $i\omega_n$  is the Matsubara frequency and  $\xi$  is the error of  $G(i\omega_n)$ ; it turns out that  $\Delta_n$  is almost constant as a function of  $n$ . The error on the energy is then estimated as the difference between the energy calculated in Eq. (7) using  $\Sigma(i\omega_n) + \Delta_n$  as the self-energy and the energy calculated using  $\Sigma(i\omega_n) - \Delta_n$  as the self-energy.

For the large value of  $U/t$  presented in Fig. 1, both approaches show good agreement in the double occupancy and in the energy, even if the energies in DCA are characterized by large error bars, due to the high-frequency tail of the self-energy.

In Fig. 2, we present the double occupancy  $D$  and the energy close to half filling, for  $n = 0.95$  and  $t' = -0.4t$ , as a function of the interaction strength  $U/t$ . We observe that the results for the double occupancies at strong coupling ( $U/t \sim 7.0$ ) and at weak coupling ( $U/t < 3.5$ ) are in good agreement, but they differ in the range  $U/t = 4-6$ . This discrepancy is related to the fact that VMC and DCA predict different values for the location of  $U_c/t$  of the metal-insulator

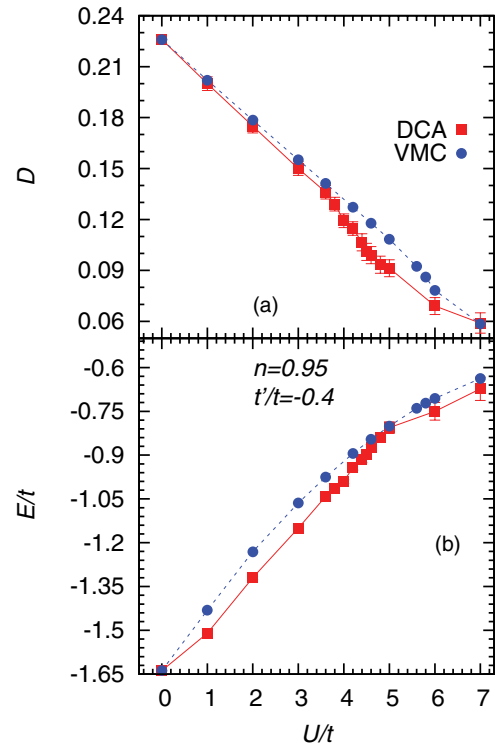


FIG. 2. (Color online) (a) Double occupancy  $D$  and (b) energy as a function of  $U/t$  for electron density  $n = 0.95$  and  $t' = -0.4t$ . Data are obtained by a VMC approach on an  $L = 162$  lattice size (blue circles) and within DCA by means of a  $2 \times 2$  plaquette in  $k$  space for a temperature  $T/t = 0.05$  (red squares). Errors in VMC are smaller than the symbol size. Lines are just guides to the eye.

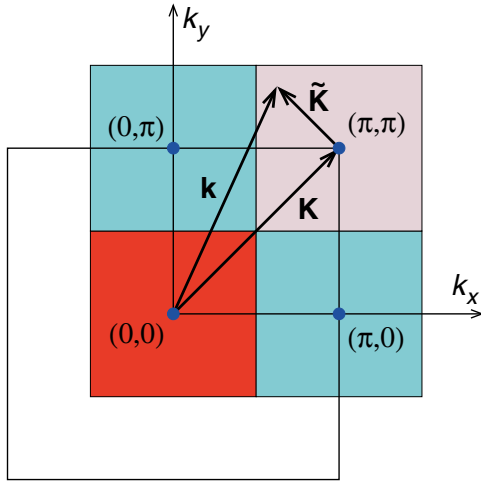


FIG. 3. (Color online) Partitioning of the square lattice Brillouin zone within the  $N_c = 4$  DCA method. There are four sectors characterized by the cluster momentum  $\mathbf{K}$ . An arbitrary reciprocal space vector  $\mathbf{k}$  is represented as a sum of  $\mathbf{K}$  and a vector  $\tilde{\mathbf{K}}$  running within the cell labeled by  $\mathbf{K}$ .

transition at half filling. The singlet RVB state is dominant in the DCA on a  $2 \times 2$  cluster, thus favoring correlated states, and also the VMC results can be slightly dependent on the accuracy of the trial wave function. The metal-insulator transition at half filling, which is weakly first order, takes place at  $U_c/t = 5.8 \pm 0.2$  within VMC,<sup>11</sup> while for DCA, on a  $2 \times 2$  cluster, the critical  $U_c/t$  is approximately estimated at  $U_c/t = 4.6 \pm 0.4$ .<sup>13,43</sup> Note that the metal-insulator transition in VMC has been determined by looking at the static structure factor  $N(q) = \langle n_{-q} n_q \rangle$ , where  $n_q = 1/\sqrt{L} \sum_{r,\sigma} e^{iqr} n_{r,\sigma}$  is the Fourier transform of the particle density. Indeed, the metallic phase is characterized by  $N(q) \sim q$  for  $q \rightarrow 0$ , which implies a vanishing gap for particle-hole excitations. On the contrary, in the insulating phase,  $N(q) \sim q^2$  for  $q \rightarrow 0$ , implying the fact that the charge gap is finite.

At difference with the double occupancies, the energy data do not show in general good agreement within the two methods. One possible reason for the discrepancy is that the energy in DCA is calculated in terms of the self-energy [see Eq. (7)], which is taken as constant within the Brillouin-zone sectors. This means that we cannot obtain a true  $k$ -dependent self-energy in our small cluster DCA calculations. Furthermore, the high-frequency part of the self-energy is evaluated according to an approximate formula that may introduce a further systematic error in the calculated self-energy. Also, VMC energies are not exact and further improvements in the wave function may lower the variational energy.

Signatures of the metal-insulator transition occurring at half filling are visible at low doping in VMC calculations, where both the double occupancy  $D$  and the energy show kinks for interactions  $U$  close to the critical  $U_c$ . Similar signatures are more difficult to infer from the DCA data around  $U/t = 4.5$  due to the larger error bars, but can be clearly observed in the behavior of the one-particle self-energy, as we discuss in the next section. In fact, both approaches, irrespective of the actual location of the MIT predicted in each method, exhibit a rapid crossover between a weak-coupling Fermi-liquid (FL)

and an intermediate to large  $U$  non-FL regime for small but finite dopings. This conclusion will be discussed in the next section, based on the observed behavior of the one-particle self-energy and of the two-particle correlation functions.

#### IV. NON-FERMI-LIQUID VERSUS FERMI-LIQUID PROPERTIES

In this section, we explore in more detail the FL and non-FL properties of the frustrated Hubbard model close to half filling, using both the VMC and DCA approaches. Long-range static correlations can be evaluated within VMC but not within DCA, due to cluster-size restrictions. Dynamical quantities like the one-particle self-energy can, however, be calculated within DCA and not with VMC; the two approaches complement each other nicely.

The nature of the non-Fermi-liquid region has been characterized, using VMC simulations,<sup>11</sup> by a strong renormalization of the underlying Fermi surface and a small violation of the Luttinger sum rule. Here, we assess the magnetic properties at low dopings via the static structure factor, defined as

$$S(q) = \frac{1}{L} \sum_{m,n} e^{iq(R_m - R_n)} \langle S_m^z S_n^z \rangle, \quad (9)$$

where  $S_m^z$  is the  $z$  component of the spin operator on site  $m$  and where  $L$  denotes the total number of sites. The presence of (short-range) antiferromagnetic correlations is signaled by the appearance of a (nondiverging) peak in  $S(q)$ , located at  $Q = (\pi, \pi)$ .

As shown in Fig. 4, for the two electron densities  $n = 0.975$  and  $n = 0.95$  at  $t'/t = -0.4$ , the non-Fermi-liquid state at  $U/t \gtrsim 6$  is characterized by antiferromagnetic correlations, which are substantially enhanced with respect to the weakly correlated metallic phase at  $U/t \lesssim 6$ . For the smaller doping,  $n = 0.975$ , the two regimes are clearly separated by a rapid increase in the value of  $S(Q)$ , which could be compatible with a first-order transition, while for the larger doping, the jump is less evident and the observed rise in the strength of the

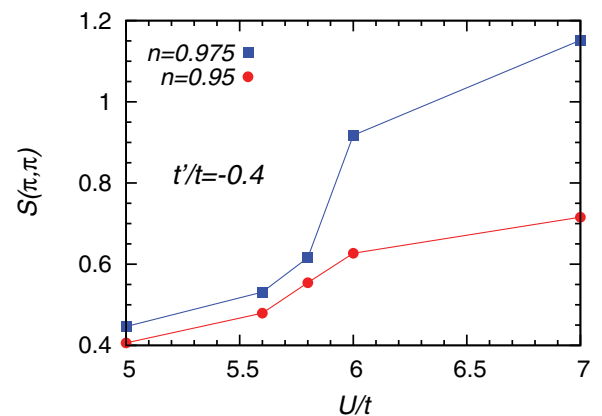


FIG. 4. (Color online) Evolution of the static structure factor correlations  $S(q) = \langle s_{-q} s_q \rangle$  at  $Q = (\pi, \pi)$  as a function of  $U/t$  for  $n = 0.975$  (blue squares) and  $n = 0.95$  (red circles) at  $t'/t = -0.4$ . The appearance of the non-FL region is characterized by a rapid increase in the short-range antiferromagnetic correlations. Data are obtained by means of VMC simulations on an  $L = 162$  lattice size.



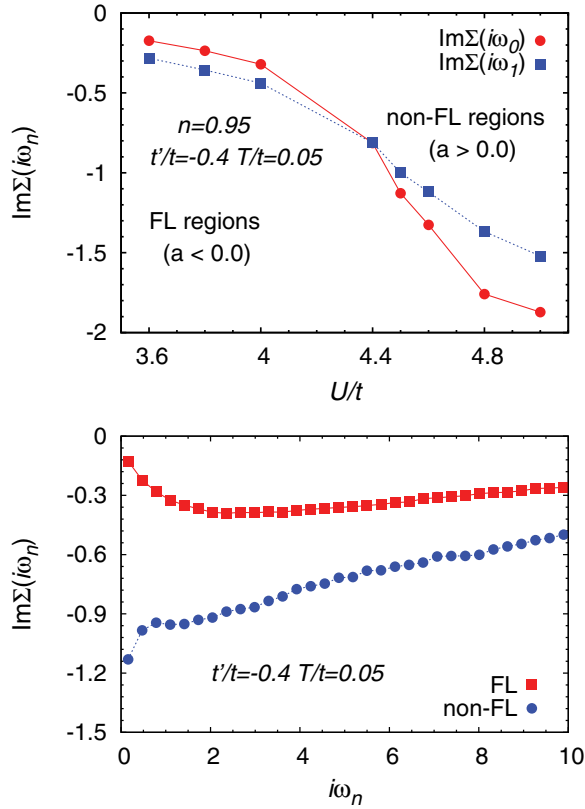


FIG. 5. (Color online) Upper panel: The imaginary part of the lowest (red circles) and the second-lowest (blue squares) self-energy values in Matsubara frequencies as a function of  $U/t$  at  $T/t = 0.05$ , with  $n = 0.95$  and  $t'/t = -0.4t$ . Data have been obtained by DCA using a  $2 \times 2$  cluster. The crossing point of both self-energies occurs around  $U/t = 4.5$ , which is the same critical  $U_c/t$  where the kink in the double occupancy data of Fig. 2 is located. The quantity  $a$  is defined in Eq. (10). Lower panel: The imaginary part of the self-energy as a function of the Matsubara frequencies at  $U/t = 3.6$  and  $n = 0.94$  (FL, red squares) and at  $U/t = 5.0$  and  $n = 0.96$  (non-FL, blue circles). Data have been obtained by DCA using a  $2 \times 2$  cluster.

short-range spin-spin correlations is more in agreement with a smooth crossover.

Next, we plot the imaginary part of the lowest and the second-lowest Matsubara frequency self-energy values as a function of  $U/t$  at  $T/t = 0.05$ ,  $n = 0.95$  and  $t'/t = -0.4t$  (see Fig. 5, upper panel), obtained using DCA. We define

$$a = \frac{\text{Im}[\Sigma(i\omega_1)] - \text{Im}[\Sigma(i\omega_0)]}{\omega_1 - \omega_0}, \quad (10)$$

where  $\text{Im}[\Sigma(i\omega_0)]$  is the imaginary part of the lowest Matsubara frequency self-energy value and  $\text{Im}[\Sigma(i\omega_1)]$  is the imaginary part of the second-lowest Matsubara self-energy value. Negative ratios  $a < 0$  indicate (quasi)-FL behavior, while positive ratios  $a > 0$  suggest a non-Fermi-liquid state. Indeed, the value of the imaginary part of the self-energy converges to zero (or to small values due to the effect of temperature) for  $i\omega_n \rightarrow 0$  in the Fermi-liquid regime, while it is monotonically decreasing for  $i\omega_n \rightarrow 0$  in the non-Fermi-liquid state; see Fig. 5, lower panel. From the data presented in Fig. 5, we find a critical  $U_c/t = 4.5$  between FL and non-FL

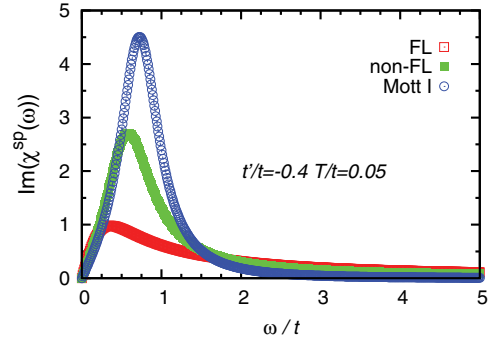


FIG. 6. (Color online) The local dynamical spin susceptibility  $\text{Im}[\chi^{\text{sp}}(\omega)]$  for  $U/t = 3.6$  and  $n = 0.94$  (FL, open red squares),  $U/t = 5.0$  and  $n = 0.96$  (non-FL, filled green squares), and  $U/t = 7.0$  and  $n = 1.0$  (Mott insulator, open blue circles), as a function of the real frequency  $\omega/t$  at  $T/t = 0.05$  and  $t' = -0.4t$ . A Padé approximation has been employed for the analytical continuation of  $\chi^{\text{sp}}(\tau)$ .

states, which is in agreement with the location of the small kink in the double occupancy  $D$ ; compare Fig. 2.

Finally, we present in Fig. 6 the local dynamical spin susceptibility  $\text{Im}[\chi^{\text{sp}}(\omega)]$  obtained within DCA with  $10^8$  QMC samplings, by performing the analytical continuation of

$$\chi^{\text{sp}}(\tau) = \langle S^z(\tau)S^z(0) \rangle, \quad (11)$$

where  $S^z = \frac{1}{2}(n_\uparrow - n_\downarrow)$  and  $\tau$  is the imaginary time, with the help of the Padé approximation. The  $\text{Im}[\chi^{\text{sp}}(\omega)]$  around  $\omega/t = 0.5$  is strongly suppressed in the FL region at  $U/t = 3.6$  and  $n = 0.94$ . This low-frequency peak is dominant in the non-FL region at  $U/t = 5.0$  and  $n = 0.96$  and in the Mott-insulating region at  $U/t = 7.0$  and  $n = 1$ . We relate the enhancement of the low-energy peak in non-FL and Mott-insulator regions to the formation of short-range antiferromagnetic correlations, as presented in Fig. 4, in terms of increased RVB-type singlet pairing. These results demonstrate the complementarity of the DCA and VMC methods in identifying the region of possible non-FL behavior, and they are compatible with studies of the Kagome and the triangular lattice.<sup>44,45</sup>

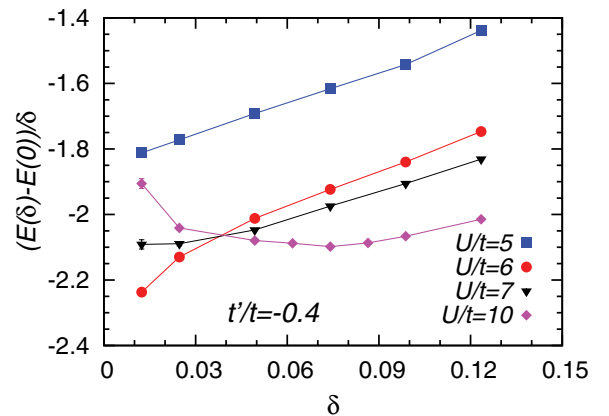


FIG. 7. (Color online) The hole energy  $E_\delta(\delta) = [E(\delta) - E(0)]/\delta$  as a function of doping for different values of  $U/t$  at  $t'/t = -0.4$ . Data are obtained by means of VMC simulations on an  $L = 162$  lattice size.

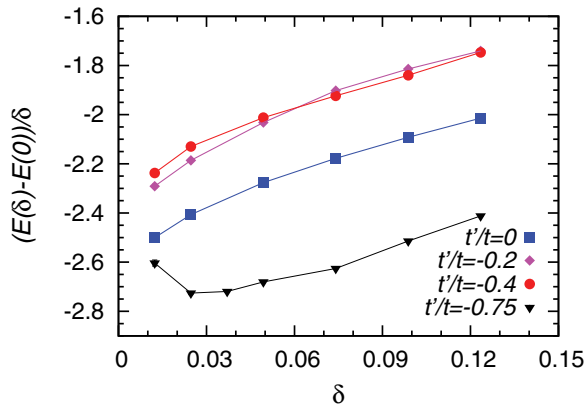


FIG. 8. (Color online) The hole energy  $E_\delta(\delta) = [E(\delta) - E(0)]/\delta$  as a function of doping for the four cases  $U/t = 6$ ,  $t'/t = 0$  (blue squares),  $U/t = 6$ ,  $t'/t = -0.2$  (pink diamonds),  $U/t = 6$ ,  $t'/t = -0.4$  (red circles), and  $U/t = 8$ ,  $t'/t = -0.75$  (black triangles). The data has been obtained by means of VMC simulations on an  $L = 162$  lattice.

## V. PHASE SEPARATION

We investigate now the possible occurrence of phase separation in the hole-doped regime  $n < 1$  by considering the hole energy defined in Eq. (1). The system is unstable to phase separation for  $\delta < \delta_c$ , if the hole energy has a minimum at a critical doping  $\delta_c$ , while a monotonically increasing hole energy corresponds, on the other hand, to an energetically favorable homogeneous solution for the doping levels investigated. Physically, phase separation is driven by magnetic correlations, which can be substantially increased, in the phase without holes, at the expense of the kinetic energy.

In Fig. 7, we focus on the case  $t'/t = -0.4$  and vary the interaction strength  $U/t$ . As expected, we find that no phase separation is possible when the half-filled case is metallic ( $U/t = 5$ ) due to the absence of a relevant magnetic energy scale. Phase separation is also not observed, interestingly, when  $U$  is only slightly above the critical interaction  $U_c$  ( $U/t = 6$ , in Fig. 7), at least for small but finite doping levels  $\delta \gtrsim 0.02$ . At very low dopings,  $\delta \lesssim 0.02$  (and  $U/t = 7$ ), phase separation could possibly be present. However, since the model is expected to exhibit a magnetic instability close to half filling, a possible phase separation occurring for  $\delta \lesssim 0.02$  would be masked by long-range magnetic order. For larger values of  $U/t$ , phase separation seems, however, to be energetically favorable for a wider range,  $\delta \lesssim 0.08$ , of doping levels. The data for larger electron repulsion ( $U/t \sim 20$ ) are not shown in Fig. 7, but they exhibit trends similar to the case  $U/t = 10$ . However, we cannot exclude that better estimates of the ground-state energy can reduce this tendency to phase separate, as detailed in Ref. 17. This is a consequence of the fact that good estimates for the energy of low-doping states are hard to obtain because of the strong local correlations.

In Fig. 8, we show the hole energy as a function of doping for four values of the next-nearest-neighbor hopping, ranging from  $t'/t = 0$  to  $t'/t = -0.75$ . The value of the Coulomb repulsion is slightly above the critical  $U_c$ , which is located between  $U/t = 5$  and  $U/t = 6$  for  $-0.4 < t'/t < 0$ , while it is located between  $U/t = 7$  and  $U/t = 8$  at  $t'/t = -0.75$ . In all of the cases relevant for the cuprates,  $t'/t \simeq [-0.1, -0.4]$ , no phase separation occurs. Only in a small range,  $\delta \lesssim 0.02$ , is a tendency for phase separation observed for  $t'/t = -0.75$ . Thus, our data suggest that for the cuprates, the Hubbard model is not unstable against phase separation when the value of the electronic repulsion is chosen to be close to the critical interaction  $U_c$  of the Mott-Hubbard transition.

## VI. CONCLUSIONS

When investigating correlated electron systems, numerical or analytical approximations are generically necessary and the accuracy of the employed approach is notoriously difficult to control. Here we compare results obtained by two complementary approaches, DCA and VMC. We find good agreement for the calculation of the double occupancies, apart from the value of the critical Hubbard  $U$  for the Mott-Hubbard metal-insulator transition at half filling, while comparing energies is more problematic, as discussed in Sec. III. We use the complementary information, i.e., static long-range correlations provided by VMC and dynamical properties provided by DCA, to investigate the physics at finite- but low-doping levels. We find that the crossover from a weakly correlated electron state at intermediate to small values of  $U$  to a non-Fermi-liquid state at intermediate to large values of  $U$  is characterized by a strong increase in local magnetic correlations. In this respect, we do not find evidence for non-Fermi-liquid properties below the critical Hubbard  $U$ , as suggested instead by a recent DCA study.<sup>12,13</sup> Our result is a solid feature of the VMC approach.<sup>11</sup> The application of DCA in the present work has been oriented to supplement the dynamical properties that are missing in VMC and we do not exclude that other studies within DCA can show evidence of non-Fermi-liquid properties also below the critical  $U$ , although this is in contradiction to VMC. This remains a controversial issue<sup>13,46</sup> and needs further study. In Sec. V, we investigate the stability of the non-Fermi-liquid state against phase separation and find it to be stable for all parameters relevant for the cuprates. These studies further prove the synergies obtainable when using complementary methods for the study of frustrated and correlated electron systems.

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