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Competing States in the t - J Model: Uniform d -Wave State versus Stripe State

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Variational studies of the t - J model on the square lattice based on infinite projected-entangled pair states confirm an extremely close competition between a uniform d -wave superconducting state and different stripe states. The site-centered stripe with an in-phase d -wave order has an equal or only slightly lower energy than the stripe with antiphase d -wave order. The optimal stripe filling is not constant but increases with J/t . A nematic anisotropy reduces the pairing amplitude and the energies of stripe phases are lowered relative to the uniform state with increasing nematicity.

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The discovery of high-temperature superconductivity in the cuprates stimulated intense study of the t - J model [1]—the strong coupling limit of the Hubbard model [2,3], on a square lattice. But open issues remain concerning the phase diagram at underdoping, especially with regard to the stability and form of stripe phases. Initially, these were considered to be simple charge- and spin-density waves with enhanced hole doping along π -domain walls in an antiferromagnetic (AF) background at a filling of one hole per unit length per stripe [4–7]. Later theoretical work found that half-filled stripes with coexisting d -wave superconducting (SC) order [8,9], or even more complex order with intertwined domain walls in both the AF and d -wave SC order [10], are very close competitors to states with uniform hole density. The proposal by Berg *et al.* [11], that the latter stripe form explained the observation by Li *et al.* [12] of two-dimensional superconductivity order over a large temperature range in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ around $x = 1/8$, stimulated further theoretical investigations. Surprisingly, many calculations on the t - J model using a range of different approximations found small energy differences between states with uniform hole density and the stripe states [10,13–16]. This near degeneracy between states with clearly different ordering suggests an underlying general physical explanation. This interpretation is further supported by the experimental observation of the stripe state in a specific hole density range in some cuprates. (See Refs. [17–23] for a review).

In this Letter, we use an improved version of the powerful infinite projected entangled-pair states (iPEPS) method on the t - J model. This method yields the lowest energy variational wave functions to date for infinite (or very large) two-dimensional systems. It gives remarkably small energy differences for the very different stripe and uniform states. Interestingly, as the accuracy of the method is increased, the energy differences between the competing states become smaller. Our version of the t - J model ignores the usual next-nearest neighbor hopping for computational simplicity, but this omission did not affect the near degeneracies in the earlier

calculations [10,14,15], suggesting an underlying general physical explanation, which remains to be uncovered.

The near degeneracy, on the one hand, makes the identification of the true ground state extremely difficult; on the other hand, it implies that the t - J model in the physically relevant regime is at or close to a phase transition between competing phases. So, small additional and/or anisotropic terms in the model can stabilize one phase over the other. Since these additional terms will depend on the particular cuprate compound, it can explain why stripes are only found in certain cuprates. As an example of a modified t - J model, we study the effect of a nematic anisotropy, which can be introduced by the tilting pattern of the CuO_6 octahedra, e.g., in the low-temperature tetragonal (LTT) phase of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ around $x = 1/8$, and can confirm that it lowers the energy of the stripe state relative to the uniform state.

Model.—The t - J model is given by the Hamiltonian

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \text{H.c.}) + J \sum_{\langle ij \rangle} \left(\hat{S}_i \hat{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right), \quad (1)$$

with $\langle ij \rangle$ nearest-neighbor pairs, $\sigma = \{\uparrow, \downarrow\}$ the spin index, $\hat{n}_i = \sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ the electron density, and \hat{S}_i the spin 1/2 operator on site i , and $\tilde{c}_{i\sigma} = \hat{c}_{i\sigma} (1 - \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma})$.

Method.—Our results are obtained with (fermionic) iPEPS—a variational tensor network ansatz to efficiently represent two-dimensional ground states in the thermodynamic limit [24–27]. It can be seen as a natural generalization of matrix product states (the underlying ansatz of the density-matrix renormalization group method [28]) to two dimensions. Originally, it was developed for spin systems and, later, was extended to fermionic systems [27,29–36]. The ansatz consists of a supercell of rank-5 tensors which is periodically repeated on the lattice. Each tensor has a physical index and four auxiliary indices which connect to the nearest-neighboring tensors. The accuracy of the ansatz can be systematically controlled by the bond dimension D of the auxiliary indices (each tensor contains $3D^4$ variational parameters). A $D = 1$ iPEPS simply corresponds to a

site-factorized wave function (product state), and by increasing D , quantum fluctuations (or entanglement) can be systematically added to the state. A similar ansatz has been employed in Ref. [37]; however, here we use a more accurate optimization scheme (the full update, cf. Ref. [27]) to find the best variational parameters. We also push the simulations to larger bond dimensions by exploiting $U(1)$ symmetries [38,39] and a more efficient contraction method (see Supplemental Material [40]).

We compare various competing low-energy states in the t - J model by using different supercell sizes in iPEPS, e.g., a uniform state with d -wave SC order coexisting with AF order at low doping, and different types of stripe states, with examples presented in Fig. 1. Each panel shows several order parameters computed with iPEPS: the hole density $\delta_i = 1 - \langle \hat{n}_i \rangle$ and the local magnetic moment \hat{S}_i^z on each site i , and the singlet pairing amplitude $\Delta = \langle \hat{c}_{i\uparrow} \hat{c}_{j\downarrow} - c_{j\downarrow} \hat{c}_{i\uparrow} \rangle / \sqrt{2}$ between neighboring sites i and j .

Uniform d -wave state.—We first discuss the results obtained with an iPEPS consisting of only two tensors, one for each sublattice, for $J/t = 0.4$. The lowest energy state we find with this ansatz has a uniform charge distribution and a d -wave SC order, coexisting with AF order at low doping (see [U] in Fig. 1). A similar state has been found in several previous studies [10,46–52]; however, here we obtain a lower variational energy for this state than the best result from fixed-node Monte Carlo (FNMC) calculations combined with two Lanczos steps (FNMC + 2L) [52], see Fig. 2(a). For example,

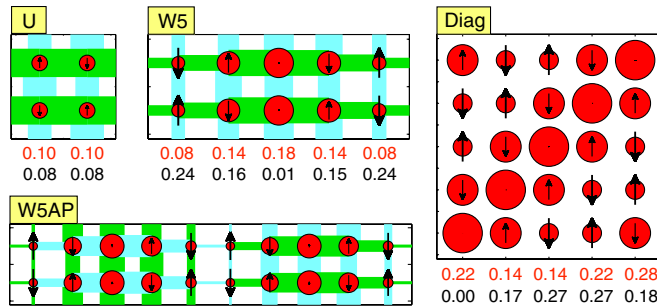


FIG. 1 (color online). Competing low-energy states in the t - J model found with iPEPS simulations using different supercells ($J/t = 0.4$). The diameter of the red dots (length of the arrows) is proportional to the local hole density (local magnetic moment) with average values given by the first (second) row of numbers below a panel. The width of a bond between two sites scales with the (singlet) pairing amplitude on the corresponding bond with a different sign in the horizontal and vertical direction indicated by the two different colors. Uniform (U) d -wave superconducting state with coexisting antiferromagnetic order ($\delta \sim 0.1$, $D = 14$), where two different tensors for the two sublattices have been used. A site-centered vertical stripe state of width $W = 5$ (W5) with in-phase d -wave order in a 5×2 supercell ($\delta \sim 1/8$, $D = 14$). A site-centered stripe state of width $W = 5$ with antiphase d -wave order (W5AP) in a 10×2 supercell ($\delta \sim 1/8$, $D = 10$). A fully-doped ($\rho_l = 1$), insulating diagonal (Diag) stripe in a $L \times L$ cell using L different tensors at a doping $\delta = 1/L$ (here $L = 5$, $D = 14$). We considered sizes up to $L = 11$.

at doping $\delta = 0.12$, we find an energy per hole $E_{\text{hole}} = (E_s - E_0)/\delta = -1.578t$ for $D = 14$, where E_s is the energy per site and $E_0 = -0.467775t$ the value at zero doping taken from Ref. [53]. This value is considerably lower than $E_{\text{hole}} = -1.546t$ obtained for a system with $N = 162$ in Ref. [52], where the energy increases with system size.

In Fig. 2(b), we present results for the singlet pairing amplitude Δ of the uniform state as a function of doping, for $D = 6$, $D = 12$, and the extrapolated data in $1/D$ (see the Supplemental Material [40] for additional data). It is suppressed with increasing D , but tends to a finite value in the infinite D limit, $\Delta \approx 0.025$ for $\delta = 0.12$. The local magnetic moment m shown in Fig. 2(c) decreases rapidly with doping, and is also suppressed with increasing D . For $\delta \lesssim 0.1$ the extrapolated value of m in $1/D$ is finite, but it vanishes for larger δ . Thus, we find coexisting d -wave and antiferromagnetic order for $\delta \lesssim 0.1$ in close agreement with previous results [10,47–52].

Stripe states.—Next we focus on vertical stripe states, which are obtained with supercells of size $P \times 2$ with P the periodicity of the stripe. Each stripe has a certain width W given by the periodicity of the charge density wave order (which is not necessarily equal to P), and a filling measured

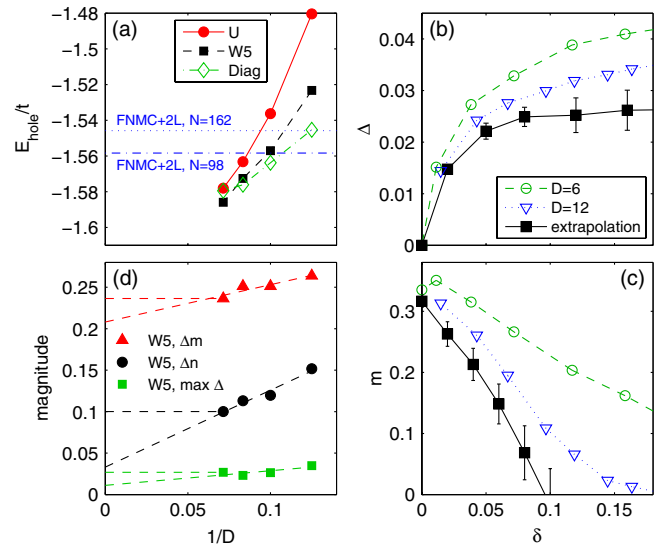


FIG. 2 (color online). (a) Energies of the competing states as a function of inverse bond dimension for $\delta = 0.12$. The horizontal lines show the best fixed-node Monte Carlo result (with two Lanczos steps) from Ref. [52]. (b)–(c) Order parameters of the uniform d -wave state as a function of doping: (b) the pairing amplitude Δ and (c) the local magnetic moment m . The extrapolated values have been obtained from a linear extrapolation of the finite D data, which provides a rough estimate of the order parameters in the infinite D limit. (d) Order parameters of the W5 stripe state as a function of inverse D for $\delta = 0.12$: the modulation strength of the local hole density $\Delta n = n_{\text{max}} - n_{\text{min}}$ and of the local magnetic moment $\Delta m = m_{\text{max}} - m_{\text{min}}$, where $n = \langle \hat{n} \rangle$ and $m = |\langle \hat{S}_z \rangle|$ are evaluated on each lattice site in the supercell. The filled squares show the maximal singlet pairing $|\Delta|$. The order parameters decrease with increasing D , but remain finite in the infinite D limit. The dashed lines are a guide to the eye.

in holes per unit length of a stripe, $\rho_l = W\delta$. In Refs. [8,37], it was found that the preferred width of a stripe increases with decreasing doping (see also the Supplemental Material [40]); i.e., depending on the doping, we need to use different supercell sizes. To simplify the discussion, we will focus on $W = 5$ stripes in the following which in our calculations are energetically favored for dopings around $\delta \sim 0.12$ [54].

The lowest energy $W = 5$ stripe we find is the W5 state shown in Fig. 1. This state exhibits a modulation in the charge-, spin-, and superconducting order, where the maximal doping is centered on a row of sites, called site-centered stripe (as opposed to bond-centered stripes, see Refs. [21,55–57] for a discussion). Figure 2(d) shows that both the amplitudes of the charge and spin modulation decrease with increasing bond dimension D but, then, tend to a finite value in the infinite D limit, which indicates that in this state the stripe order persists in this limit.

The d -wave pairing in the W5 stripe state has the same sign structure on neighboring stripes, i.e., in-phase order. In agreement with previous studies [10,13–15,58,59], we also find a competing low-energy state which has antiphase order (W5AP in a 10×2 supercell shown in Fig. 1) with an energy per hole that is only slightly higher (of the order of $0.001t$ for $D = 10$) than the in-phase stripe; see the Supplemental Material [40] for additional data. Since the energy difference between the two states is very small, it is conceivable that antiphase stripes get stabilized by additional terms (such as a next-nearest neighbor hopping [10]). This further supports the proposal that antiphase ordered stripes are the reason for the lack of 3D superconductivity above $T = 4$ K in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ around $x = 1/8$ [12,60], because they lead to a suppression of the interlayer Josephson coupling between the copper-oxygen planes [11].

Finally, we also find diagonal stripes with a low energy, e.g., the state shown in the right panel in Fig. 1. These states are obtained by using supercells of size $L \times L$ with L different tensors arranged in a diagonal stripe pattern. These stripes are insulating and have a filling of $\rho_l = 1$ holes per unit length. However, we will show in the next section that diagonal stripes are energetically unfavorable at large D .

Uniform vs stripe states.—So far, we have found various low energy states in different supercells. Next, we make a systematic comparison of their energies for $J/t = 0.4$ and $\delta = 0.12$, to determine which of the competing states is the true ground state. For a fixed value of $D = 8$ we find that the uniform state has a higher variational energy than the W5 stripe state, in agreement with previous findings [37]. Furthermore, it turns out that diagonal, insulating stripes—which were not considered in Ref. [37]—are even lower in energy for $D = 8$. However, from this we cannot conclude that the diagonal stripe state is the ground state, but we must examine how the energies of the competing states change upon increasing D , shown in Fig. 2(a): All energies decrease with increasing D , however, with different slopes, such that the W5 stripe state becomes lower in energy than the diagonal stripe state for $D > 12$. For $D = 14$, the W5 stripe state has

the lowest energy, but since the energy of the uniform state decreases faster (at least for $D < 12$) than the energy of the W5 state, it may get lower (or equal) in the large D limit. Such a crossing of energies of competing states as a function of D has already been found in another model [61], and it is also a possible scenario for the present case.

Even if we cannot conclusively determine the ground state based on our results, the important message from our data is that the uniform and the vertical stripe state are still strongly competing at considerably lower variational energies than in previous studies for large 2D systems [52]. Thus, it seems likely that both states play an important role for the low-energy physics of the t - J model, and that small perturbations (e.g., disorder, open boundaries [62], etc.) in the system can be enough to stabilize different states. However, our data shows that diagonal stripes are energetically higher than vertical stripes. (We have not found evidence for the stable diagonal stripes observed in experiments [19,63] in the low doping limit in the present model.)

Remarks on phase separation.—While it is well established that the t - J model undergoes phase separation for large J/t and small doping [64–69], some previous studies predicted phase separation to occur also in the physically relevant regime $J/t \sim 0.4$ (see, e.g., [48,70]). In our study, we do not find evidence for phase separation, at least not in the doping regime $\delta \gtrsim 0.08$ (see the Supplemental Material [40] for a discussion).

Other values of J/t .—It is conceivable that the close competition between the uniform and the vertical stripe state may be a specific feature for $J/t = 0.4$. This motivated us to do a similar study for other values of J/t also to check whether we can detect a clear phase transition between the two states as a function of J/t . However, for small values $J/t = 0.2$ as well as for large values $J/t = 0.8$, we find a qualitatively similar dependence on D as in the $J/t = 0.4$ case; i.e., the uniform state is higher than the stripe state, but they become closer and closer with increasing D . Thus, the strong competition between the two states can be found for a wide range of J/t . We also computed the pairing amplitude as a function of J/t , shown in Fig. 3(a) for $\delta = 0.14$, which increases with J/t for both states, with almost a linear dependence for the uniform state.

A rather unexpected finding concerns the optimal stripe filling, i.e., the filling at which the energy per hole has a minimum for a stripe of a fixed width. Several previous studies predicted that the minimum is at $\rho_l = 0.5$ holes per unit length (i.e., half-filled stripes) [8,9,16,37,71], which is in close agreement with our results for $J/t = 0.4$. However, here we find that this is only true for $J/t \sim 0.4$, and that the optimal stripe filling actually depends continuously on J/t ; i.e., it is a function of the physical parameters of the system. Figure 3(b) shows that, for $J/t = 0.2$, the optimal ρ_l is ≈ 0.35 , i.e., smaller than half filling, whereas for $J/t = 0.8$ the minimum energy per hole is found for a fully doped stripe ($\rho_l = 1$).

Nematic case.—Motivated by the fourfold rotational lattice symmetry breaking in each CuO_2 layer in the LTT phase of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ and related compounds

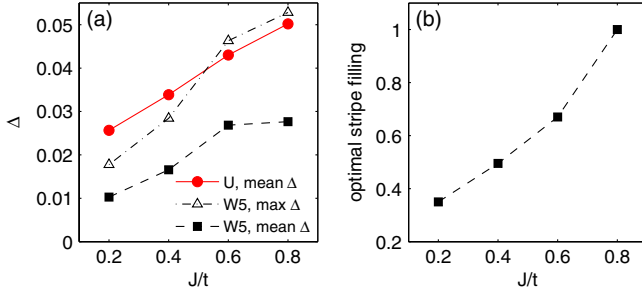


FIG. 3 (color online). (a) Pairing amplitude as a function of J/t for $\delta = 0.14$, $D = 10$. (b) Optimal stripe filling $\rho_l = W\delta$ as a function of J/t ($D = 10$, $W = 5$).

around $x = 1/8$ we study the effect of a nematic anisotropy in the t - J model. In Fig. 4(a), we show the results for $t_x = 0.85t_y$ and $J_x = (0.85)^2J_y$ with $J_y/t_y = 0.4$, at a doping $\delta = 0.1$. Comparing this with the isotropic case, the vertical W5 stripe state has lowered its energy with respect to the uniform state, which shows that nematicity helps to stabilize the stripe state, in agreement with previous findings [72–74]. We also find that the optimal stripe filling is shifted toward smaller doping, around $\rho_l \approx 0.4$; see the Supplemental Material [40].

At low doping, the preferred orientation of the stripe is along the direction with stronger couplings, i.e., the y direction, in this case, as found in Refs. [73–75] (and in Ref. [72] for nonsuperconducting stripes). However, we find that at large doping ($\delta \gtrsim 0.14$) it is the opposite orientation which is preferred, i.e., horizontal stripes. This can be understood by looking at the energy contributions in the two spacial directions in the isotropic case (see the Supplemental Material [40] for the individual energy contributions): For a vertical stripe around half filling, the exchange term E^J is dominant over the kinetic term E^{kin} , and it is stronger (lower) in the y than in the x direction, $E_y^{\text{kin}} < E_x^{\text{kin}}$. Thus, in the nematic case, the stripe can minimize its energy by orienting itself *parallel* to the direction with stronger couplings. However, for large δ it is the transverse kinetic energy E_x^{kin} which is dominant, since with increasing doping, E^J becomes weaker. Furthermore,

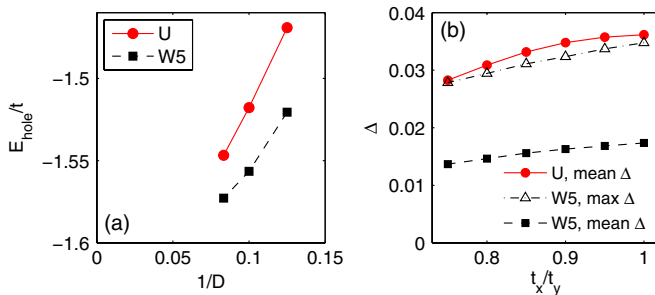


FIG. 4 (color online). (a) Energies as a function of inverse bond dimension for $\delta = 0.1$ in the nematic t - J model with $J/t = 0.4$ and $t_x = 0.85t_y$. (b) The pairing amplitude of the uniform state decreases with increasing nematicity (here $(t_x + t_y)/2 = 1$ and $(J_x/t_x + J_y/t_y)/2 = 0.4$ are kept constant, $\delta = 0.13$, $D = 8$).

$E_x^J < E_y^J$ at large doping, so that for the total energy we find $E_x^{\text{tot}} < E_y^{\text{tot}}$. Thus, in the nematic case at large doping it is favorable for the stripe to form perpendicular to the direction with stronger couplings. (A similar conclusion for fully doped stripes has been reached in Ref. [72].)

Finally, we study the effect of the nematicity on the pairing amplitude, shown in Fig. 4(b). For both the uniform and the stripe state we find that the pairing amplitude is suppressed with increasing nematicity; i.e., the maximal pairing is obtained in the isotropic case.

Conclusion.—Even with a substantially higher accuracy than in previous studies, and in the limit of an infinite system where boundary and finite size effects are negligible, we still find an extremely close competition between the uniform and the vertical stripe state. The origin of this near degeneracy remains a crucial open question and requires further theoretical investigation. One possibility is that the nearest-neighbor t - J model is at or close to a phase transition which separates the two states; i.e., small additional terms in the Hamiltonian can be enough to stabilize one of the states. These additional terms depend on the particular cuprate compound, and we believe that studying the effect of these terms will explain why stripes appear in certain materials whereas other compounds show no signs of stripes. For example, here we confirmed that a nematic anisotropy, which can be found in the LTT phase of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, favors the stripe state over the uniform state.

We have studied the properties of the competing states individually: the uniform state has d -wave order coexisting with antiferromagnetic order for $\delta \lesssim 0.1$. The pairing amplitude increases with J/t approximately linearly and gets suppressed with increasing nematicity. The vertical stripe state is site-centered and has a finite modulation amplitude of the spin and charge order. Stripes with antiphase order have a similar or only slightly higher energy than stripes with in-phase order. In the presence of a nematic anisotropy, the stripe orientation depends on the doping. Finally, we have shown that the optimal stripe filling is not necessarily $\rho_l = 0.5$, but depends on J/t . Therefore, a theory of the physics of stripes should include the optimal stripe filling as a free parameter.

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