$t-J_z$ model on the Cayley tree and the square lattice

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Candidates for the ground state of the anisotropic $t-J_z$ model at low hole doping are studied within two related lattices: the Cayley tree and the square lattice. The Cayley tree allows for the evaluation of the single hole as well as the hole-pair ground states to arbitrary precision. Threshold values for the formation of bound hole pairs appear to be similar for both lattices. We show that the main contributions to the binding of a hole pair on the Cayley tree comes from the excess number of frustrated bonds ("spinons"). Considering systems with a larger number of holes, we establish high stability of configurations with holes forming straight domain walls between nonequivalent antiferromagnetic domains. In particular, for the Cayley tree we find that domain-wall-like configurations have lower energy than separate hole pairs. For the square lattice, however, there exists at low but finite doping a parameter interval 0.18 < J/t < 0.56 where, in the ground state, holes are paired.

I. INTRODUCTION

The phase diagrams of several models for strongly correlated electrons have been studied very extensively in past years in connection with the search for the microscopic mechanism of superconductivity at high temperatures. Both prototype models, the Hubbard model and the t-J model,¹ remain a challenge in this respect. In particular, the question still remains open whether there exists a phase with paired electrons in the physically relevant regime of parameters and at low concentration of holes doped into the reference antiferromagnet (AFM).

The phase diagram of the t-J model is best understood in one dimension, where the strong superconducting (SC) pairing fluctuations are restricted to the vicinity of the phase separated region at $J \gg t^2$. Recently it has been shown that an external staggered field h > 0 introduces into one dimension several characteristic features of $D \ge 2$ systems.³ It can induce the existence of bound hole pairs and dominant SC pairing fluctuations at J < t far from the phase separation. This one-dimensional (1D) model offers a simple qualitative as well as quantitative explanation for the origin and the threshold for hole-pair formation, observed before at $J \gtrsim 0.2t$ in the (zero-field) model on a square lattice via the exact diagonalization study of 4×4 system,⁴ recently confirmed for systems with N = 26 sites, ^{5,6} as well as by the Monte Carlo technique.⁷ Extending these findings to systems with a larger number of holes or at finite hole concentration, there still remains a controversy whether a bound hole pair is a precursor of (a) a phase with paired holes (electrons),⁸ (b) the (physically less appealing) cluster formation, related to the phase separation into the hole-rich and spin-rich phases, 9^{-11} or (c) the striped (charge-density wave) phase with holes forming domain walls (DW's) in an AFM.^{12,13} The evidence for the stability of the latter phase has been found in a recent numerical study of the t-J model on the square lattice with N = 26 sites,⁵ where the lower threshold for the inhomogeneous phase with DW formation appears at $J \sim 1.4t$ much below the usual phase separation,

i.e., the cluster instability at $J \gtrsim 2.5t$.

In this paper we investigate the t- J_z model with the anisotropic (Ising-like) spin exchange, defined by

$$H = -t \sum_{\langle ij \rangle_s} (c_{js}^{\dagger} c_{is} + \text{H.c.}) + J \sum_{\langle ij \rangle} (S_j^z S_i^z - \frac{1}{4} n_j n_i) , \qquad (1)$$

where $c_{is}^{\dagger}(c_{is})$ are projected fermionic operators, taking into account that double occupancy of sites is not allowed. n_i and S_i are the corresponding local fermion number and spin operators, respectively.

In comparison with the isotropic t-J model, the t-J_z model represents a substantial simplification near half filling. Namely, in the system with half-filled band without added holes the ground state is a trivial Néel state (for J > 0), while in the isotropic model spin fluctuations destroy the long-range order in one dimension and substantially decrease the staggered magnetization in two dimensions.¹⁴ In a macroscopic system a finite number of holes cannot destroy the AFM order in the t- J_z model, while effects in the t-J model are more subtle due to long-wavelength AFM magnons. Nevertheless, there are several important similarities between results in both models. In particular, the mechanism that leads to the bound state of two holes, first clearly established in the isotropic model on the 2D square lattice,⁴ seems to be qualitatively the same for the anisotropic model. The latter fact has been confirmed by variational calculations,¹⁵ the perturbation expansion,¹⁶ and most transparently in the 1D model with an external staggered field.³

The t- J_z model offers a possibility to study numerically in more detail systems with more holes, $N_h > 2$, which are essential for the understanding of the possible phases at finite hole doping. Although in general the complete basis set to describe the system ground state is not reduced relative to the isotropic t-J model, there are several controlled approximations allowing for reliable quantitative results. In particular, the calculations are simple on the Cayley tree, where one can obtain numerically accurate results for the ground-state energies for $N_h = 1$ as

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well as for $N_h = 2$ (this paper). Although results for $N_h > 2$ and the hole DW's cannot be obtained to the same precision, still they are relatively more accurate than for the square lattice.

The organization of the paper is as follows. In Sec. II we address the problem of two holes on a Cayley tree. In Sec. III we consider holes forming a domain wall both on the Cayley tree and on the square lattice. We conclude the paper (Sec. IV) by summarizing our results and commenting briefly on their implications.

II. HOLE PAIRS ON CAYLEY TREE

We are interested in the ground state of few holes in the AFM ordered spin background. On the Cayley tree (of coordination number z + 1) it is easy to achieve the AFM-Néel order (coordination) in the reference system without holes by imposing on the final Nth level (see Fig. 1) the boundary condition with all spins aligned. Few holes added to such system cannot destroy the long-range AFM order. In addition, we assume that boundaries repel holes and therefore consider only ground states with holes confined to the bulk of the tree.

In the t- J_z model (1) the reference system without holes has a simple Néel order. The ground state of a single hole $N_h = 1$ introduced into the bulk of the AFM, can be treated analytically since the hole can perform only retraceable paths. The ground-state energy $\epsilon_1 = E_1 - E_0$ has been first obtained by Brinkman and Rice¹⁷ with the result $\epsilon_1 = \sqrt{z(z+1)t}$ for J = 0. General J > 0 requires the solution of a system of linear equations

$$(\epsilon_1 - V_0)\alpha_0 = \sqrt{z} + 1t\alpha_1 ,$$

$$(\epsilon_1 - V_1)\alpha_1 = \sqrt{z+1}t\alpha_0 + \sqrt{z}t\alpha_2 ,$$

$$(\epsilon_1 - V_n)\alpha_n = \sqrt{z}t\alpha_{n-1} + \sqrt{z}t\alpha_{n+1}, n > 1 ,$$

(2)

with the stringlike potential¹⁸

$$V_n = [z + 2 + (z - 1)n - \delta_n] \frac{J}{2} .$$
(3)

The calculation of the ground state for two holes $N_h = 2$ is much more involved due to the importance of the fermionic signs and due to a number of possible candidates for the hole-pair wave functions having different symmetries. We will investigate here only a particular pair



FIG. 1. Cayley tree with branching z = 3. Dots represent the spins in the AFM (Néel) ordered state. Crosses denote overturned spins relative to the Néel state, while the wavy line denotes the spin-string between holes.

eigenstate, which can evolve from a hole pair introduced into the AFM background at the tree root, i.e., with the two holes initially on levels 0 and 1, respectively. Starting with such initial condition only wave functions can develop which are symmetric in single-hole positions within the same tree level.

It is convenient to introduce normalized basis functions, characterized in general with three levels $r \le m < n$, m,n denoting levels of both holes, while r is the highest common root for both holes. An example is shown in Fig. 1. Single-hole hopping in an AFM background leaves behind a string of overturned spins and the second hole following the first one can erase the string. It is easy to verify that the length of the spin string, and consequently the potential energy, is determined solely by the level of the root r and both hole levels m,n. Basis functions can be written as

$$|rmn\rangle = \frac{1}{\sqrt{(z-1)^{n+m-r-2}}} \sum_{i_r \mu \nu} a^+_{m\mu} a^+_{n\nu} \tau^+_{\mu\nu} |0\rangle ,$$
$$0 < r < m < n , \quad (4a)$$

$$|rrn\rangle \frac{1}{\sqrt{z^{n-1}}} \sum_{i_{r}\nu} a_{ri_{r}}^{+} a_{n\nu}^{+} \tau_{i_{r}\nu}^{+} |0\rangle, \quad r < n$$
 (4b)

Here, spinless fermionic operators $a_{m\mu}^+$ represent the hole creation at position μ within the level *m*, acting on the reference Néel state $|0\rangle$. $\tau_{\mu\nu}^+$ is a bosonic operator creating a spin string between positions $m\mu$ and $n\nu$ with the common root at ri_r . In (4a) the sum runs over all the positions $\mu(r), \nu(r)$ within respective levels *m*, *n*, which can be reached from the highest common root at ri_r .

From the construction (4) of basis states, representing the complete set only for the chosen initial condition, it is evident that both holes cannot enter the same level, i.e., m < n. Hole-pair states (4) and Hamiltonian matrix elements have also the translation symmetry with respect to levels r = 1, N of the Cayley tree. So it is natural to assume that the ground state will be for $N \rightarrow \infty$ characterized with the wave vector q = 0, the eigenfunction $|\Psi_0\rangle$ being of the form

$$|\Psi_{0}\rangle = \frac{1}{\sqrt{N}} \sum_{r\bar{m}\bar{n}} \alpha_{\bar{m}\bar{n}} |r, r + \bar{m}, r + \bar{n}\rangle .$$
(5)

Within this reduced set of basis functions it is now straightforward to find the matrix elements using the Hamiltonian (1),

$$\begin{split} H_{\tilde{m}\tilde{n}}^{\tilde{m}\tilde{n}} &= E_0 + (z+1)J + \frac{z-1}{2}(\tilde{m}+\tilde{n}-1)J - \frac{1}{2}J\delta_{\tilde{n}-1} , \\ H_{0\tilde{n}}^{0,\tilde{n}+1} &= -(1+\sqrt{z})t, \quad H_{\tilde{m}\tilde{n}}^{\tilde{m},\tilde{n}+1} &= -\sqrt{z}t, \quad \tilde{m} > 0 , \\ H_{0\tilde{n}}^{1\tilde{n}} &= -\sqrt{z-1}t, \tilde{n} > 1, \quad H_{\tilde{m}\tilde{n}}^{\tilde{m}+1,\tilde{n}} &= -\sqrt{z}t, \quad \tilde{n} > \tilde{m} + 1 . \end{split}$$
(6)

Within the diagonal term $H_{\bar{m}\bar{n}}^{\bar{m}\bar{n}}$ the third term is the spinstring contribution. The last term leads to an additional contact attraction between holes on NN sites and is due to the known fact that two close holes break one exchange bond less than two separate holes. It is easy to diagonalize the Hamiltonian matrix (6) for particular z, J and find numerically hole-pair energies ϵ_2 to high precision. Here we will consider only the tree with z = 3 which simulates the branching in the square lattice. In this case larger N, e.g., N > 20, are needed only for J < 0.1t, still we can show that on approaching $J \rightarrow 0$ $\epsilon_2 = 2\epsilon_1$. Results for the pair binding energy $\epsilon_b = \epsilon_2 - 2\epsilon_1$ at general J > 0 are presented in Fig. 2. It follows that hole pairs are bound for $J > J_c \sim 0.28t$. We note that this threshold J_c is very close to the one obtained for the $t - J_z$ model (see Sec. III and Refs. 19 and 20) as well as for the isotropic t - J model on the square lattice. ^{5,6}

Due to differences between the square lattice and the Cayley tree the symmetry of such hole-pair state cannot be directly related to 2D states, still the closest correspondence is with the q = 0 and the mixture of p and d rotational states on the square lattice. [Note, that unlike for the isotropic model, the ground state (g.s.) of the $t-J_z$ model on square lattice for two holes is p-wave-like²⁰ in the parameter region here considered.] At present, we cannot prove that there are no other bulk hole-pair solutions (ignoring possible surface states) with lower ϵ_2 . These other candidates correspond to different initial conditions and are less symmetric, hence also more difficult to study. We have tested some candidates, however no indication for a more stable solution was found.

To conclude this section let us comment again on the origin of binding. As has been already pointed out by the present authors³ in the case of the one-dimensional $t-J_z$ model in a staggered field h, the state of paired holes becomes energetically favorable relative to two separate holes for some $J > J_c(h)$, due to the energy cost J, which arises from two additional spinons for separate holes. Below we show that this *same* effect lies at the origin of binding of holes on the Cayley tree as well, where the staggered field is provided by the AFM background.



FIG. 2. Hole-pair binding energy ϵ_b (full line) vs J/t for the Cayley tree. Contributions to ϵ_b [see Eq. (9)] are also plotted: $\delta \langle T \rangle$ (dashed line), $\delta \langle V_s \rangle$ (dot-dashed line), the spinon contribution $\epsilon_{\rm sp}$ (long-dashed line), and the broken-bond contribution $\epsilon_{\rm bb}$ (dotted line). Here and in subsequent figures the energies are measured in units of t.

First note that by diagonalizing the Hamiltonian matrices, defined by Eqs. (2), (3), and (6), for one and two holes, respectively, one obtains also the ground-state (g.s.) amplitudes $\{\alpha_n\}$ and $\{\alpha_{\bar{m}\bar{n}}\}$. Then the g.s. energy can be calculated as a sum of contributions from different pieces of the Hamiltonian. In the two-hole case one has

$$\epsilon_2 = -\frac{J}{2}\alpha_{0,1}^2 + \langle T_2 \rangle + \langle V_s \rangle , \qquad (7)$$

where the first term represents the contribution from the broken bond, the second term is the kinetic energy contribution, and the last term is the g.s. expectation value of the string potential $V(l)=l(z-1)J/2, l=\tilde{m}+\tilde{n}-1\geq 0$. Similarly, for the single hole

$$\epsilon_1 = \frac{J}{2} (1 - \alpha_2^2) + \langle T_1 \rangle + \langle V_s \rangle , \qquad (8)$$

where the second and third contribution are of the same origin as for two holes. The first term, however, results from the *extra* frustrated bond (analog of a spinon in one dimension) generated at the origin of the string as soon as the hole hops away from it. Then, the overall contribution to the binding energy is

$$\epsilon_{b} = \delta \langle T \rangle + \delta \langle V_{s} \rangle + \epsilon_{bb} + \epsilon_{sp} , \qquad (9)$$

$$\epsilon_{bb} = -\frac{J}{2} \alpha_{0,1}^{2}, \quad \epsilon_{sp} = -J(1 - \alpha_{0}^{2}) .$$

There are several important features to be noted. First, the contribution from broken bond ϵ_{bb} is seen to be relevant only for $J/t \gtrsim 1.5$, whereas for the physically relevant region $J/t \leq 0.5$ it is completely dominated by the spinon contribution ϵ_{sp} . Indeed, for $J/t \leq 0.5$ (see Fig. 2) the holes are well separated from each other and the contact interaction induced via the broken bond becomes *irrelevant*. The kinetic energy contribution $\delta \langle T \rangle$ is always positive and almost constant, except for very small J/t (for very long strings), where the $\frac{2}{3}$ -power law becomes manifest. This is because hopping of two holes tied by a string is suppressed, due to interference effects. as compared to a single hole, and consequently $\langle T_2 \rangle > 2 \langle T_1 \rangle$. Finally, the string contribution is also positive and comparable in magnitude to $\delta \langle T \rangle$ for $J/t \leq t$, but negligible otherwise. The explanation for this lies in the fact that there are more states in the pairedhole case with a given string length than for the isolated hole, thus resulting in a larger $\langle V_s \rangle$.

III. HOLES FORMING DOMAIN WALLS

When a finite concentration of holes is introduced into the system, there are several possibilities how pair formation for $N_h = 2$ would affect the situation with $N_h >> 1$. One possible scenario is that holes would form a domain wall separating two different AFM domains. An indication for the latter has been found recently in the numerical investigation of the *t-J* model with more $(N_h = 4)$ holes.⁵ This scenario represents also a natural extension of the 1D *t-J* model, where the ground state for a single hole (holon) represents a DW in AFM correlated background spins.

A. Cayley tree

Due to the presence of many mobile holes, the quantum problem of a dynamical DW formed by holes is a difficult one, even on a Cayley tree. We are not able to solve it exactly, but still to a high degree of accuracy (not for very small $J/t \ll 1$). By appropriate boundary conditions for spins it is easy to simulate the basic configuration on the Cayley tree (see Fig. 3), where holes form a DW between two different AFM domains. Our aim is to find the energy of such many-body states, after we allow also for all quantum fluctuations, i.e., all possible hole excursions with the t- J_z model.

Let us first consider a simplified problem, where in a DW only a single (tagged) hole is allowed to hop (see Fig. 3), while the others stay fixed within the DW. This problem can be as well considered as a mean-field-like approximation (MFA) to the many-body DW dynamics. The search for the ground state is equivalent to the problem of a single particle (hole) hopping in the potential

$$\widetilde{V}_{n} = [z + (z - 1)|n|] \frac{J}{2} , \qquad (10)$$

where *n* denotes the hole position with respect to the DW, while *z* should be odd and $z \ge 3$ for the meaningful definition of DW. In the spirit of MFA we have attributed to a single hole only a part of the potential energy $\tilde{V}_0 = zJ$ of the basic DW configuration.

Further on we will discuss only the z=3 case. Note that \tilde{V}_n is smaller than V_n for all *n* for a single hole in a homogeneous AFM, Eq. (3). On the other hand, a hole in the DW is restricted in hopping due to neighboring holes, e.g., $H_0^1 = -\sqrt{2}t$ (for symmetrized basis with $n \ge 0$) in contrast to $H_0^1 = -2t$, Eq. (2), for an isolated hole in an AFM. Numerical results for the energy $\epsilon_{\rm DW}$ of the tagged hole in a DW, representing also the MFA energy (per hole) for the many-hole DW, are presented in Fig. 4. They can be compared to ϵ_1 , as introduced in Sec. II. We notice that for J > 0.2t one gets $\epsilon_{\rm DW} < \epsilon_1$, being already a strong indication for the high stability of DW configurations.

 $\epsilon_{\rm DW}$ represents a reasonable approximation to the true DW energy $\tilde{\epsilon}_{\rm DW}$ (per hole). Since the exact evaluation of $\tilde{\epsilon}_{\rm DW}$ would require essentially the complete many-body basis of the t- J_z model, we perform only the diagonalization within the restricted basis of hole and spin configurations. In particular, we use the following restrictions: (a) we consider the DW of finite length L (see Fig.



FIG. 3. Domain-wall configuration on a Cayley tree.



FIG. 4. Energies of the single mobile hole on a Cayley tree: (a) ϵ_{DW} , in the domain wall (\bullet), i.e., MFA DW energy per hole, and (b) ϵ_1 , in a homogeneous AFM (\bigcirc).

3), but extended by periodic boundary conditions, (b) the hole can perform only a single lateral hop (left or right) along the DW direction, and (c) in the vertical direction (on Fig. 3) holes can hop at most the distance M (up or down). We notice that the ground-state energy is much more sensitive to changes in M than to those of L, so we perform the calculation on the systems up to L = 4 and M = 4. This yields already ~ 30 000 basis states, requiring the use of the Lanczos diagonalization procedure. Results of such variational method seem to converge well for J > 0.3t, while for smaller J deviations become more pronounced.

In Fig. 5 we present results for the DW condensation energy (per hole) $\Delta = \tilde{\epsilon}_{DW} - \epsilon_2/2$, calculated with respect to separate hole pairs. A rather striking conclusion is, that in the whole regime $J > J_c$ separate hole pairs are unstable against the formation of a hole DW. Some simple arguments can be given to interpret this result: (a) holes in a DW profit from a reduced string potential, Eq.



FIG. 5. Domain-wall condensation energy Δ (\bullet) vs J/t for the Cayley tree. The hole-pair binding energy ϵ_b (\bigcirc) is replotted for comparison.





FIG. 6. Domain-wall configuration on a square lattice.

(10), the effect pronounced to its extremum in a 1D chain (z=1), and (b) a separate bound hole pair gains only a part of the coherent kinetic energy, while a hole in the DW also keeps at least the 1D kinetic energy contribution.

B. Square lattice

We approach the analysis of a hole-DW on a square lattice, separating two different AFM domains, in the same way as above. We first consider the DW where a single (tagged) hole is mobile, as presented in Fig. 6. The evaluation of the ground-state energy for this system is more involved (due to the absence of translational invariance in one direction) than finding accurately the states of a single hole. In order to simplify the problem somewhat, we neglect all hole excursions containing loops or crossings. Then it is easy to devise a numerical method to evaluate successively energies of configurations with different hole paths. Approximately they are proportional to the spin-string length n, and qualitatively similar to \tilde{V}_n in Eq. (10).

Again, we choose the potential energy of the hole in the reference DW configuration as in Eq. (10), so that the calculated ϵ_{DW} can be interpreted as the DW energy per hole within MFA. In Fig. 7 we compare results for ϵ_{DW} with the energy ϵ_1 of a single hole in a homogeneous AFM, as calculated from the diagonalization of the N=26 system.

Results for the square lattice, Fig. 7, and for the Cayley tree, Fig. 5, have common features, but also essential



FIG. 7. Energies of the single mobile hole on a square lattice: (a) ϵ_{DW} , in the domain wall (\bullet), i.e., MFA DW energy per hole, and (b) ϵ_1 , in a homogeneous AFM (\odot).



FIG. 8. Single-hole paths on a square lattice taken into account in the variational calculation.

differences. At larger J/t holes in a DW are clearly more stable than separate holes. However, on a square lattice critical value $J \sim 0.5t$ appears substantially higher than on the Cayley tree. Moreover, $\epsilon_{\rm DW}$ does not approach the same value as ϵ_1 for $J \rightarrow 0$. This seems to result from different connectivity of the Cayley tree with respect to the square lattice, on which the hole moving in the vicinity of the DW is restricted in motion (to half-plane) also for longer paths, while on the Cayley tree this is not the case.

The analysis of the complete many-body DW problem is much more involved. Namely in comparison with the DW on a Cayley tree where holes following different neighboring vertical branches do not interact, there is a number of restrictions on the motion of holes in the square lattice. We approach the problem by constructing the variational wave functions using the following procedure and simplifications: (a) we consider a system with the length up to L = 4 with periodic conditions, (b) we allow for each hole up to $M_p = 35$ different paths, half of them presented in Fig. 8, (c) considering interfering paths of different holes we omit all configurations which are not reachable in a unique way, i.e., have possible exchange of holes, involve path crossings, etc., (d) diagonal energies for allowed configurations are calculated exactly, and (e) due to the large basis, i.e., up to L^{M_p} states, the Lanczos diagonalization is used to find the ground state.

Results obtained in this way seem to be reliable in the regime J > 0.3t, and are shown in Fig. 9, together with ϵ_b



FIG. 9. Domain-wall condensation energy Δ (•) vs J/t for the square lattice. The hole-pair binding energy ϵ_b (\bigcirc) is plotted for comparison.

as obtained in Refs. 19 and 20. Although the hole DW appears stable well below J = t, the critical value being $\tilde{J}_c \sim 0.56t$, still there exists a clear window of stable separate hole pairs $J_c \approx 0.18t < J < \tilde{J}_c$. This is consistent with the MFA result in Fig. 7, albeit there remains only the quantitative agreement between the MFA result and the many-body DW analysis.

IV. CONCLUSIONS

In this paper we analyzed the phase diagram of the anisotropic t- J_z model in the limit of low hole doping. Both lattices considered, the Cayley tree and the square lattice, show common features. In particular, ground-state properties of the single hole and of the hole pair introduced into the reference AFM agree even quantitatively for both lattices, at least outside the Nagaoka regime, i.e., $J \gtrsim 0.1t$. The hole motion is governed by the spin-string effects. While the single hole motion is (approximately) incoherent, the hole pair retains a part of coherent propagation (e.g., for the p state along one direction only²⁰).

On the Cayley tree the origin of low hole-binding threshold $J_c \sim 0.28t$ is seen to result from essentially two contributions, the hole-pair kinetic energy due to coherent propagation, favoring separate holes, and the spinon (string-end contribution), favoring the bound hole pair. From the discussion presented at the end of Sec. II, it is clear that within the same, i.e., retraceable path approximation, the above picture should equally well apply to a hole pair on a square lattice. Taking into account loops, which can form on a square lattice, is expected to play no significant role since cancellation in contributions from kinetic energy and string potential V_s to ϵ_b will again occur. Moreover, the relative weight of such configurations in the g.s. becomes negligible for long(er) strings. Likewise, inclusion of spin fluctuations should not alter the above picture in any essential way, as results also from numerical calculations.^{5,6} Namely, close to the pairing instability hopping of holes occurs on a scale much faster than that of spin fluctuations, i.e., holes hop against a quasistatic spin background, and except for extra spinons and the excess kinetic energy, cancellation of contributions to ϵ_b should occur.

At low but finite hole doping we have to compare different competing states, corresponding to different phases. It appears that configurations with holes forming DW between (two) nonequivalent AFM domains are surprisingly stable, both in the Cayley tree and in the square lattice. The origin of the low energy of such states can be explained by the fact that holes in a DW profit from the reduced number of broken exchange bonds while they still keep low kinetic energy due to weakly

perturbed (predominantly 1D) motion perpendicular to the DW. Such configurations can be as well regarded as a coupled system of chains with a single holon (hole in a AFM DW) within each chain. Due to the AFM background displacements of holes on different chains become coupled, however the total energy remains quite competitive with the system with separate hole pairs. In this respect both lattices seem to differ. While on the Cayley tree hole DW appear to be more stable than separate hole pairs, the square lattice allows for an intermediate phase with a gas of bound hole pairs. The origin of this discrepancy seems to be in different connectivity of both lattices. High stability of DW solutions at finite doping is not unexpected, since similar conclusions were reached (solutions representing charge-density waves and spindensity waves with regular DW arrangements) within the Hartree-Fock analysis of the Hubbard model at low doping. 12, 13

We did not consider in this paper the instability towards formation of larger hole droplets (consisting of more than two holes), which would represent at finite doping the instability to the usual phase separation into the hole-rich and spin-rich phase.⁹⁻¹¹ From our previous results on the 1D t-J-h model³ as well as on the 2D t-J model,⁵ it follows that clustering wins only at larger J, typically J > 2t, and the relevant driving mechanism seems to be simply due to reduced number of bonds in a cluster. This phenomenon appears outside the relevant regime J < t with competing phases of paired holes and hole-DW configurations, respectively. Most other analytical and numerical approaches to the problem of the phase separation in the 2D t-J model do not clearly distinguish between clustering and possible DW formation, so their results should be interpreted with care.

We expect great similarity between the phase diagrams of the t- J_r model and the isotropic t-J model. The thresholds for hole binding on the 2D square lattice have been recently found to be quite close numerically. 5,6,19,20 Also the onset of hole droplets should only depend on the interplay between the strength of exchange bond and the kinetic energy. The question is how would spin fluctuations in the t-J model influence the relative stability of the hole pairs and hole-DW configurations. It has been found by the present authors by means of the perturbation expansion in t/J that spin fluctuations increase substantially the binding energy of the hole pair.¹⁶ On the other hand, we do not expect any substantial influence of quantum fluctuations and reduced AFM ordering on the hole motion and its potential energy within the DW. Hence, we would claim an enhanced regime of hole pairing in the 2D isotropic t-J model, consistent with numerical evidence in Ref. 5.

- ¹For a review see, e.g., T. M. Rice, in *High Temperature Super-conductivity*, Proceedings of the 39th Scottish Universities Summer School in Physics, edited by D. P. Turnstall and W. Barford (Hilger, London, 1991), p. 317.
- ²M. Ogata, M. Luchini, S. Sorella, and F. F. Assaad, Phys. Rev. Lett. 66, 2388 (1991).
- ³J. Bonča, P. Prelovšek, I. Sega, H. Q. Lin, and D. K. Campbell, Phys. Rev. Lett. **69**, 526 (1992); P. Prelovšek, I. Sega, J. Bonča, H. Q. Lin, and D. K. Campbell, Phys. Rev. **47**, 12 224 (1993).
- ⁴J. Bonča, P. Prelovšk, and I. Sega, Phys. Rev. B **39**, 7074 (1989); Y. Hasegawa and D. Poilblanc, *ibid.* **40**, 9035 (1989).

⁵P. Prelovšek and X. Zotos, Phys. Rev. B 47, 5984 (1993).

- ⁶D. Poilblanc, Phys. Rev. **48**, 3368 (1993). Note that contrary to the previous reference, results for $N_h \leq 2$ on a cluster of 26 sites on a square lattice were obtained within the unrestricted basis.
- ⁷M. Boninsegni and E. Manousakis, Phys. Rev. B **47**, 11897 (1993).
- ⁸E. Dagotto and J. Riera, Phys. Rev. Lett. 70, 682 (1993).
- ⁹V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. 64, 475 (1990); S. A. Kivelson, V. J. Emery, and H. Q. Lin, Phys. Rev. B 42, 6523 (1990).
- ¹⁰W. O. Putikka, M. U. Luchini, and T. M. Rice, Phys. Rev. Lett. 68, 538 (1992).
- ¹¹R. Valenti and C. Gros, Phys. Rev. Lett. 68, 2402 (1992).

- ¹²H. J. Schulz, Phys. Rev. Lett. 64, 1445 (1990).
- ¹³D. Poilblanc and T. M. Rice, Phys. Rev. B 39, 9749 (1989).
- ¹⁴E. Manousakis, Rev. Mod. Phys. 63, 1 (1991).
- ¹⁵B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **60**, 740 (1988); R. Eder, Phys. Rev. B **45**, 319 (1992).
- ¹⁶P. Prelovšek, I. Sega, and J. Bonča, Phys. Rev. B **42**, 10706 (1990).
- ¹⁷W. F. Brinkman and T. M. Rice, Phys. Rev. B 2, 1324 (1970).
- ¹⁸L. N. Bulaevskii, E. L. Nagaev, and D. L. Khomskii, Zh. Eksp. Teor. Fiz. **54**, 1562 (1968) [Sov. Phys. JETP **27**, 836 (1968)]; S. A. Trugman, Phys. Rev. B **37**, 1597 (1988).
- ¹⁹J. Riera and E. Dagotto, Phys. Rev. B 47, 15 346 (1993).
- ²⁰P. Prelovšek and I. Sega (unpublished).