Effective approach to the Nagaoka regime of the two dimensional $t$–$J$ model

M. M. Maška and M. Mierzejewski  
Department of Theoretical Physics, Institute of Physics, University of Silesia, 40–007 Katowice, Poland

E. A. Kochetov  
Theoretical Physics Laboratory, Joint Institute for Nuclear Research, 141980 Dubna, Russia

L. Vidmar  
J. Stefan Institute, SI-1000 Ljubljana, Slovenia

J. Bonča  
J. Stefan Institute, SI-1000 Ljubljana, Slovenia and  
Department of Physics, FMF, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia

O. P. Sushkov  
School of Physics, University of New South Wales, 2052 Sydney, Australia

We argue that the $t$–$J$ model and the recently proposed Ising version of this model give the same physical picture of the Nagaoka regime for $J/t \ll 1$. In particular, both models are shown to give compatible results for a single Nagaoka polaron as well as for a Nagaoka bipolaron. When compared to the standard $t$–$J$ or $t$–$J_z$ models, the Ising version allows for a numerical analysis on much larger clusters by means of classical Monte Carlo simulations. Taking the advantage of this fact, we study the low doping regime of $t$–$J$ model for $J/t \ll 1$ and show that the ground state exhibits phase separation into hole–rich ferromagnetic (FM) and hole–depleted antiferromagnetic (AFM) regions. This picture holds true up to a threshold concentration of holes, $\delta \leq \delta_t \simeq 0.44 \sqrt{J/t}$. Analytical calculations show that $\delta_t = \sqrt{J/2\pi t}$.

I. INTRODUCTION

It is by and large recognized that the key properties of high-temperature superconducting materials can be explained with the help of the two-dimensional $t$–$J$ model. Therefore, the major interest is focused on this model in the regime that seems to be relevant to high-temperature superconductivity. Since the Hubbard on-site repulsion $U$ in cuprates is usually assumed to be an order of magnitude bigger than the hopping integral $t$, the relevant AFM coupling between nearest neighbor sites $J = 4t^2/U$ is about tenths of $t$.

Much less is known about the $t$–$J$ model in the small–$J$ limit, i.e., the large–$U$ limit of the Hubbard model. At half filling the infinite–$U$ Hubbard model has AFM ground state. However, in 1965 Nagaoka proved a theorem which states that when exactly one hole is introduced the ground state becomes FM. In the infinite–$U$ limit the ground state of the half filled Hubbard model is macroscopically degenerate. When a single hole is introduced this degeneracy is lifted, since it is energetically favorable for the hole to move in a background of fully aligned spins. A simple proof of Nagaoka’s theorem was later given by Tasaki, who also showed that additional density-dependent interactions do not alter this result.

The Nagaoka theorem is one of very few rigorous results concerning strongly correlated electronic systems. However, it does not say anything about the case of a finite density of holes as well as finite AFM interaction. The question of a character of the leading instability of the Nagaoka state with respect to the AFM exchange term or finite density of holes has attracted much interest. For finite $J$ ($J > 0$) and/or finite doping the ground state is determined by the competition between antiferromagnetism favored by the exchange interaction and Nagaoka’s ferromagnetism favored by the kinetic energy. This competition presumably drives the system into two phases, a hole-rich FM region where the kinetic energy is minimized and a region with localized electrons characterized by AFM order. Generally, the $t$–$J$ model may display different types of phase separation depending on the value of $J/t$ and the actual state of affairs is far from being clear. It was demonstrated in Refs. that phase separation takes place in the $t$–$J$ model for all values of $J$. Other authors find phase separation only for large $J$. It is very difficult to establish unambiguously the presence or absence of phase separation in the small–$J$ limit of the $t$–$J$ model. The main reason is that a high-accuracy, unbiased calculation of the ground state energy as a function of the hole density is required to assess the competition between the interaction and kinetic energies. The spatial inhomogeneity in the phase separated state makes analytical approaches rather involved.

On the other hand, since the FM bubbles are relatively large it is difficult to apply numerical approaches like the quantum Monte Carlo method or exact diagonalization. In this situation, a computational method that is able to tackle a system sufficiently large to describe the spatially separated state in the small–$J$ limit of the $t$–$J$ model is required.
In this paper, we demonstrate that Monte Carlo simulations for the recently proposed Ising version of the $t$–$J$ model provide sound and reliable results in this limiting case. We employ this approach to study the formation of a bubble of the FM phase when holes are introduced into an AFM background. Namely, we investigate the so-called Nagaoka polaron which sets in for vanishing doping and $J/t \ll 1$. The Nagaoka polaron represents an intermediate state between the homogeneous FM Nagaoka ground state for $J = 0$ and the standard spin polaron for $J > 0.2$. Numerical studies of the Nagaoka polaron are difficult because of its large spatial dimensions: for $J \rightarrow 0$ its radius diverges as $J^{-1/4}$.

In this paper we formulate an effective description of the Nagaoka regime, which is based on the recently proposed Ising version of the $t$–$J$ model. In the subsequent sections we recall the basic properties of this model and explain why it gives the same physical picture of the Nagaoka regime as the standard isotropic $t$–$J$ model. These qualitative arguments are accompanied by quantitative comparison with the numerical results for the isotropic model. For the reader convenience we first recall density matrix renormalization group (DMRG) studies on the Nagaoka polaron. We then present new results for the Nagaoka bipolaron, studied in the $t$–$J$ model by means of exact diagonalization in the limited functional space (EDLFS).

Numerical calculations within the Ising version are by far less demanding hence much bigger clusters and/or much larger doping become accessible. After having successfully tested the single and two–holes cases, we investigate the ground state properties of the $t$–$J$ model ($J/t \ll 1$) doped with several holes. In particular, we show that all holes are confined in a single FM polaron. We discuss how its energy and spatial dimensions depend on the number of holes. For low hole densities, our results provide an evidence that the leading instability of the FM Nagaoka state is a phase separation rather that a single spin flip.

II. THE ISING $t$–$J$ MODEL

We start with the $t$–$J$ Hamiltonian on a square lattice

$$H_{t-J} = -\sum_{ij\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + J \sum_{\langle ij \rangle} \left( Q_i Q_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right),$$

where $\hat{c}_{i\sigma} = P c_{i\sigma} P = c_{i\sigma}(1-n_{i\sigma})$ is the projected electron operator (to exclude the on-site double occupancy), $Q_i = \sum_{\sigma,\sigma'} c_{i\sigma} \tau_{\sigma\sigma'} c_{i\sigma'}$, $\tau^2 = 3/4$, is the electron spin operator and $\hat{n}_i = P n_i P = n_{i\uparrow} + n_{i\downarrow} - 2 n_{i\uparrow} n_{i\downarrow}$ is the projected electron number operator. Hamiltonian (1) contains a kinetic term with the hopping integrals $t_{ij}$ and a potential $J$ describing the strength of the nearest neighbor spin exchange interaction. At every lattice site the Gutzwiller projection operator $P = \prod_i (1-n_{i\sigma}(1-n_{i\sigma}))$ projects out the doubly occupied states. Physically this modification of the original Hilbert space results in strong electron correlation effects.

At the low-energy scale of order $J \ll t$, it is reasonable to consider the background spin configuration to be nearly frozen with respect to the hole dynamics. In this case the properties of the low-energy quasiparticle excitations in the $t$–$J$ model are at least qualitatively similar to those in the anisotropic $t$–$J_z$ model, in which the spin-flip part of the Heisenberg interaction is dropped:

$$H_{t-J_z} = -\sum_{ij\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + J_z \sum_{\langle ij \rangle} \left( Q_i^z Q_j^z - \frac{1}{4} \hat{n}_i \hat{n}_j \right),$$

The global continuous spin SU(2) symmetry of the $t$–$J$ model now reduces to the global discrete $Z_2$ symmetry of the $t$–$J_z$ model. Although $Q_i^z Q_j^z$ interaction possesses discrete $Z_2$ symmetry, the original SU(2) symmetry of all other terms of the Hamiltonian is preserved. Therefore, the symmetry of the $t$–$J_z$ model depends on whether $J_z$ is zero or finite. Namely, for $J_z = 0$ the SU(2) symmetry is restored again. Although this model is more amenable to numerical calculations, again only rather small lattice clusters are allowed.

One may hope that the full Ising version of the $t$–$J$ model in which the $t$-term also possesses the global discrete $Z_2$ spin symmetry results in a more tractable though still nontrivial model. It by definition has the global discrete $Z_2$ symmetry, regardless of the values of the incoming parameters. This implies that the resulting system can be thought of as a doped classical Ising model. However, it is not clear how such a model can be derived directly from (1), since the projected electron operators $\hat{c}_{i\sigma}$ transform themselves in the fundamental representation of SU(2). To overcome this problem, the recently proposed spin-dopon representation of the projected electron operators can be used.

The idea behind that approach is to assign fermion operators $d_{i\sigma}$ to doped carriers (holes, for example) rather than to the lattice electrons. The enlarged on-site Hilbert space is spanned by the state vectors $|\sigma a\rangle$, with $\sigma = \uparrow, \downarrow$ labeling the 2D Hilbert space of the lattice spin, $S_i$, and $a = 0, \uparrow, \downarrow, \uparrow\downarrow$ labeling the 4D on-site dopon Hilbert space. The physical space consists of the spin-up $|\uparrow\rangle$, spin-down $|\downarrow\rangle$ and spinless vacancy $|\uparrow\downarrow\rangle$ and spinless vacancy $|\uparrow\downarrow\rangle$. The remaining unphysical states are removed by the constraint

$$S_i M_i + \frac{3}{4} n_i^d = 0,$$

where $M_i = \sum_{\sigma,\sigma'} d_{i\sigma}^\dagger \tau_{\sigma\sigma'} d_{i\sigma'}$ stands for the dopon spin operator so that

$$Q_i = S_i + M_i.$$
In view of the relation $(S^\alpha)^2 = 1/4$, the constraint (3) can equivalently be written in the form
\[ \sum_{\alpha=x,y,z} S^\alpha_i M^\alpha_i + n^d_i \sum_{\alpha=x,y,z} (S^\alpha_i)^2 = 0. \] (5)
Within the full Ising $t$–$J$ model, one should have $Q^\pm_i = Q^\pm_i \equiv 0$. In view of Eq. (4), this requires $S^\pm_i = M^\pm_i = 0$. To explicitly derive the Ising $t$–$J$ model, we therefore project the dopon operators onto the Hilbert space singled out by the local constraint
\[ S^z_i M^z_i + \frac{1}{4} n^d_i = 0. \] (6)
which can be thought of as an "Ising" form of Eq. (3). It represents the $Z_2$ singlet under the $Q^i \rightarrow \pm Q^i$ transformations $\in Z \subset SU(2)$. The physical electron projected operators reduce to the $Z_2$ spinors:
\[ \tilde{c}_{i\downarrow} = \mathcal{P}_{ph} d_{i\uparrow}^\dagger \mathcal{P}_{ph} = \left( \frac{1}{2} - S^z_i \right) d_{i\uparrow}, \] (7)
\[ \tilde{c}_{i\uparrow} = \mathcal{P}_{ph} d_{i\downarrow}^\dagger \mathcal{P}_{ph} = \left( \frac{1}{2} + S^z_i \right) d_{i\downarrow}, \] (8)
with the projection operator $\mathcal{P}_{ph} = 1 - (2S^z_i M^z_i + n^d_i/2)$. It can readily be checked that
\[ Q^+_i = \frac{1}{2} (\tilde{c}_{i\uparrow}^\dagger \tilde{c}_{i\downarrow} - \tilde{c}_{i\downarrow}^\dagger \tilde{c}_{i\uparrow}) = S^z_i + M^z_i, \]
\[ Q^-_i = (Q^+_i)^\dagger = \tilde{c}_{i\uparrow}^\dagger \tilde{c}_{i\downarrow} \equiv 0, \]
as desired: the transverse components of the electron spin operators no longer appear in the theory.

The underlying onsite Hilbert space rearranges itself in the following way. The operators (7) act on the Hilbert space $\mathcal{H}_i = \{|\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$. These operators do not mix up any other states. Operator $\tilde{c}_{i\downarrow}$ destroys the spin-down electron and creates a vacancy. This vacancy is described by the state $|\downarrow\downarrow\rangle$. The similar consideration holds for the $\tilde{c}_{i\uparrow}$ operators. Now, however, the vacancy is described by the state $|\uparrow\downarrow\rangle$. Those two vacancy states are related by the $Z_2$ transformation. The operator $(Q^+_i)^2 = \frac{1}{4} (1 - n^d_i)$ produces zero upon acting on both states. The physical Hilbert state is therefore a direct sum $\mathcal{H}_{ph} = \mathcal{H}_\uparrow \oplus \mathcal{H}_\downarrow$. Under the $Z_2$ transformation ($\uparrow \leftrightarrow \downarrow$, $S^y_i \rightarrow -S^y_i$) we get $\mathcal{H}_\uparrow \leftrightarrow \mathcal{H}_\downarrow$, which results in $\mathcal{H}_{ph} \rightarrow \mathcal{H}_{ph}$. In the isotropic $t$–$J$ model these two 2D spaces merge into a 3D SU(2) invariant physical space, where the vacancy is just an antisymmetric linear combination given by the SU(2) spin singlet, $|\uparrow\downarrow\rangle_i = \left( |\uparrow\downarrow\rangle_i - |\downarrow\uparrow\rangle_i \right)/\sqrt{2}$. The symmetric combination splits off, since it represents an unphysical spin-triplet state.

As a result, one arrives at the representation (2) in which, however, the electron projection operators are given by Eqs. (7). All the parts of this Hamiltonian possess the global discrete $Z_2$ symmetry whereas the global continuous SU(2) symmetry is completely lost. Close to half-filling, the Ising $t$–$J$ Hamiltonian takes on the form:
\[ H^{sing}_{t-J} = \sum_{ij\sigma} t_{ij} d_{i\sigma}^\dagger d_{j\sigma} + J \sum_{(ij)} \left[ \left( S^z_i S^z_j - \frac{1}{4} \right) \\
+ S^x_i M^x_j + S^y_i M^y_j \right], \] (9)
which is to be accompanied by the constraint (6). The magnetic $M^x_j M^x_j$ term has been dropped as being small of order $\delta^2$ in the limit $\delta := \langle n_d \rangle \ll 1$.

In practical calculations, we find convenient to implement the constraint (6) with the help of a Lagrange multiplier. Since $S^z_i M^z_i + n^d_i/4 \geq 0$, the global Lagrange multiplier
\[ \lambda \sum_i \left( S^z_i M^z_i + \frac{1}{4} n^d_i \right) \] (10)
enforces the constraint (6) locally. The unphysical occupancy of an arbitrary site would enhance the total energy by $\lambda \rightarrow +\infty$. Therefore, all unphysical on-site states are automatically eliminated, so that the local constraint is taken into account rigorously.

The main difference between the $t$–$J_z$ and Ising $t$–$J$ models originates from the different symmetries of the hopping terms as discussed in. The one-hole energy obtained for the isotropic $t$–$J$ model is shown to be in between the results obtained for the $t$–$J_z$ and Ising models. In the regime $J \ll t$, the differences between $t$–$J$ and $t$–$J_z$ models are comparable to those between $t$–$J$ and Ising models.

A. Monte Carlo approach

The Hamiltonian (9) together with the constraint (10) describe a system that contains both classical (S) and quantum (d) degrees of freedom. However, there is no direct interaction between the quantum particles. Therefore, the Ising $t$–$J$ model is closely related to a (multi-component) Falicov–Kimball model and we can apply an efficient Monte Carlo (MC) approach derived exclusively for the latter model. This numerical approach can be applied neither to the standard $t$–$J$ model nor to the $t$–$J_z$ one. In the latter case one should use the SU(2) invariant constraint (3) which involves $S^\pm$ operators.

The classical MC method has already been applied to the Ising $t$–$J$ model in order to study dynamics of holes and destruction of the AFM order with increasing hole concentration. Here, however, we are not interested in the thermodynamics of the system, but rather in its ground state properties. Therefore, the Metropolis algorithm is used for simulated annealing. And once again, since simulations are performed by random walk through the configuration space of the classical variables, there is no need for quantum annealing and relatively large lattices can be studied. The size of the lattice for a given
$J/t$ and a given number of holes is adjusted so that the size of the polaron be always significantly smaller. Since the holes can propagate only within the FM region, the finite size effects become negligible. Most of the calculations are carried out on $20 \times 20$ and $30 \times 30$ lattices, but in some cases larger clusters, up to $50 \times 50$ are necessary as well. From now on, a value of the nearest neighbor hopping amplitude is used as the energy unit ($t_{ij} = t = 1$ for $i$ and $j$ being nearest neighbors and $t_{ij} = 0$ otherwise).

III. TEST OF A SINGLE POLARON PROBLEM

Neglecting the spin–flip term is generally a crude approximation, hence the standard and the Ising $t$–$J$ models describe very different systems. However, we will show that for vanishing doping and small $J$ both approaches give rise to the same physical picture of the Nagaoka polaron.

The density matrix renormalization group (DMRG) studies\cite{18} of the 2D $t$–$J$ model have shown that for $J < 0.03$ the Nagaoka polaron is indeed stable. Its size and energy can be determined by balancing the kinetic energy of a hole freely propagating within a FM bubble against the magnetic energy of the FM bubble relative to the energy of the Néel state. Minimizing the sum of these two energies one easily finds expressions for the radius $R$ and energy $E$ of the Nagaoka polaron (see Ref. \cite{18}):

$$R \approx 1.12 J^{-1/4}, \quad E \approx -4 + 9.2 \sqrt{J},$$

which for $J < 0.03$ accurately fit the DMRG data.

The Ising $t$–$J$ model displays essentially the same physics. The constraint (10) allows for propagation of holes only within static FM bubbles where $S_j^z = -M_i^z$ and formation of these bubbles takes place at the expense of the exchange interaction, which favors AFM alignment of $S_j^z$. In both models the magnetic energy of a bubble is qualitatively similar and is proportional to $J$ multiplied by the number of FM bonds. Qualitative differences should arise from different energies per bond of the Néel ground state of the undoped systems. Figs. 1 and 2 show quantitative comparison of both models. Here, we show the ground state properties of a single Nagaoka polaron in the Ising $t$–$J$ model for a $50 \times 50$ system with periodic boundary conditions and $\lambda = 300$. The radius and energy of the Nagaoka polaron have been compared with expressions (11) as well as with the bare DMRG data for the SU(2) $t$–$J$ model taken from Ref. \cite{18}. The overall agreement is clearly visible.

To conclude this section, we notice that the Ising $t$–$J$ model provides a simple and reasonably accurate description of a single Nagaoka polarons for $J \ll 1$ simply because the spin–flip term becomes irrelevant inside a sufficiently large FM bubble which confines the movement of holes.

IV. THE NAGAOKA BIPOLARON PROBLEM

In the preceding section we have successfully tested the case of a single carrier doped into Mott insulator. Since our aim is to study a system at finite doping such a test might still be insufficient. Therefore, we investigate also the system doped with two holes. On the one hand it is a first nontrivial step towards understanding the spatial hole distribution in doped systems (uniform versus inhomogeneous). On the other hand, due to large spatial
dimensions of the Nagaoka polaron, it is already a challenging problem for fully quantum numerical approaches.

To investigate the Nagaoka bipolaron in the isotropic $t$–$J$ model, we employ the EDLFS method. This method describes properties of carrier/carriers doped into a planar ordered antiferromagnet.\footnote{One starts from a translationally invariant state of two carriers in the Néel background}

$$|\phi_0\rangle_p = \sum_\gamma (-1)^{M(\gamma)} c_0 c_\gamma |\text{Neel}\rangle,$$

(12)

where the sum runs over two nearest neighbors to site 0 and $M(\gamma)$ sets the appropriate sign to generate $p_\gamma$-wave symmetry. The kinetic part $H_k$ as well as the off–

Then, the ground state $|\Psi_0\rangle$ is calculated within the limited functional space by means of the Lanczos method. The advantage of EDLFS over the standard exact diagonalization (ED) approach follows from systematic generation of selected states which contain spin excitations in the vicinity of the carriers. It enables investigation of much larger systems, which is particularly important in the Nagaoka regime. We apply this method and study the average distance $D$ between two holes in the $t$–$J$ model.

From the construction of EDLFS follows that $N_h$ determines maximum distance between holes and spin excitations as well as the maximum accessible $D$. Therefore, all characteristic length–scales of investigated problem should be smaller than a certain $\xi(N_h)$. Since the successive application of the nearest neighbor hopping [see Eq. (13)] closely resembles the random walking process we expect that $\xi(N_h) \propto \sqrt{N_h}$. The numerical complexity of the two–holes problem allows us to study $N_h$ up to 12. Therefore, for small $J$ we carry out a finite size scaling with respect to the size of the Hilbert space and study $D(J) \equiv D(J, N_h \to \infty)$. The finite size effects should vanish when $\xi(N_h)/D(J) \gg 1$ or equivalently $N_h/D^2(J) \gg 1$. We have found that this vanishing can universally be described by the Gaussian:

$$D(J) - D(J, N_h) = \alpha \exp \left\{ -\beta \left[ \frac{N_h}{D^2(J)} \right]^{2.5} \right\},$$

(14)

where parameters $\alpha$ and $\beta$ are independent of $J$. Note that for a given $J$ fitting of $D(J, N_h)$ involves only a single free parameter $D(J)$ which simultaneously represents the extrapolated distance between two holes. Fig. 3 shows the extrapolation, while the resulting $D(J)$ is shown in Fig. 4. Finally, the quality and the universality of the finite–size scaling is directly shown in Fig. 5. One can clearly see that all data for $J = 0.04, \ldots, 0.14$ merge into a single curve, which strongly supports the assumptions behind Eq. (14). This also demonstrates a self–consistency of the approach.

These results provide solution of the long–standing open problem, i.e., whether two holes in the $t$–$J$ model form a bound state in the small $J$ limit.\footnote{Since $D(J) > 3.5$ for $J < 0.10$, the problem can hardly be solved by exact diagonalization on 32–site cluster\footnote{where the maximal possible distance between two holes is 4 lattice spacings. Note that the symmetry of the bound state is $p$–wave for $J \lesssim 0.15$. Therefore, the results using the EDLFS method indicate that two holes in the single band $t$–$J$ model are always bound, which may not necessarily be the case in more general models describing the CuO$_2$ plane.}.
The most important result shown in Fig. 4 concerns the power-law dependence:

\[ D(J) \simeq 1.93J^{-0.27}, \tag{15} \]

hence \( D(J) \) is roughly proportional to the radius of a single-hole polaron \( R(J) \) [see Eq. (11)]. Already this result suggests that the linear dimensions of polaron and bipolaron are determined by the same mechanisms, which are properly captured by the Ising \( t-J \) model. In order to show that this expectation holds true we have calculated \( D \) in the Ising version of the \( t-J \) model. Results are shown as (red) stars in Fig. 6. In the same figure results for the \( t-J \) model are presented as (blue) dots. One can clearly see that the distance between holes \( D \) in the Ising \( t-J \) model increases with decreasing \( J \) slower than in the full \( t-J \) model. This result is not a surprise: in the isotropic \( t-J \) model (as well as in the \( t-J_z \) one) a hole is able to enter the AFM surrounding of the FM bubble. Since the boundary of the FM bubble is unpenetrable in the Ising \( t-J \) model, we expect a smaller average distance between holes in the latter case. However, it turns out that the difference has only a quantitative character, i.e., only the coefficient in Eq. (15) is approx. 33% smaller. This agreement shows that these two methods, i.e., the EDLFS method for the full \( t-J \) model and the MC method for the Ising \( t-J \) model are complementary in a sense: The applicability of the EDLFS method is limited by the maximum size of the Hilbert space, and since the distance between holes increases with decreasing \( J \), this method cannot be used when \( J \) is too small. On the other hand, the importance of the spin–flip term in the \( t-J \) Hamiltonian diminishes with decreasing \( J \) and the approximation that leads to the Ising \( t-J \) model becomes more reliable in the region where the EDLFS method cannot be applied any longer. The main advantage of the Ising \( t-J \) model is that it can be studied within the framework of the classical MC method on clusters sufficiently large to describe large polarons that emerge at small \( J \).

V. FINITE HOLE DENSITY

Up to this point we have been analyzing one and two holes in the whole system. Since the size of the (bi)polaron and its energy do not depend on the size of the lattice [provided the lattice is significantly larger than the (bi)polaron size], these results effectively describe the case of the vanishing density of holes. Then, the important question arises as to how the ground state of the Ising \( t-J \) model evolves when the number of holes increases. Possible scenarios include phase separation or homogeneous distribution of holes. It is also possible that a single polaron becomes unstable at some critical value of the hole number giving way to smaller polarons.

In order to study this problem we calculate the total energy of the system as a function of the number of holes \( E(N) \). Convex \( E(N) \) for some \( N \) indicates that it is energetically favorable to split a FM bubble with \( N \) holes into smaller bubbles with \( M < N \) holes, provided that \( E(M) \) is concave. If \( E(N) \) is convex for arbitrary \( N \), holes will not form polarons with more than one hole. On the other hand, if \( E(N) \) is concave for arbitrary \( N \), all holes introduced into the system will gather in a single FM region. In other words, the phase separation into a hole–rich FM region and an AFM region without holes takes place.

Accurate determination of \( E(N) \) is generally a difficult task. For \( N = 1 \) the shape of the polaron is almost circular, but for higher \( N \) the geometry becomes nontriv-
Fig. 7 shows the Nagaoka polarons and corresponding hole wave functions for $N = 2, \ldots, 5$. The shape of the polaron follows directly from the spatial structure of the occupied orbitals. The diagonal orientation of almost rectangular polarons minimizes the magnetic energy along the line between FM and AFM regions.

With increasing $N$ the size of the FM bubble increases, so a large lattice is necessary to avoid the finite size effects. The advantage of the Ising version of the $t$–$J$ model becomes evident, since it can be reliably investigated on lattices much larger than those accessible to the fully quantum methods like quantum MC, exact diagonalization or even EDLFS. Using larger lattices we study polarons containing up to 10 holes. In Fig. 8 we show the polaron energy $E(N)$ as a function of the number of holes $N$ for $J = 0.01$. Studying other values of $J$ from 0.01 to 0.1 (not shown) we fitted the energy with a function $E(N) = aN + b\sqrt{N}$. In Sec. V.A we justify such a form of $E(N)$. We have found that in all cases $b$ is positive, which means that $E(N)$ is concave. This in turn implies that the Ising version of $t$–$J$ model displays a phase separation for all those values of $J$ at which it is still equivalent to the isotropic $t$–$J$ model.

An important question concerns the fraction of the system occupied by each of the magnetic phases. It can be answered by comparing the size of the polaron to the size of the whole system. Fig. 9 shows the relation between the fraction of the lattice sites with ferromagnetically aligned spins $N_p/N_s$ and the density of holes $\delta = N/N_s$. $N_p$ is the number of lattice sites in the polaron and $N_s$ is the size of the lattice. This dependence can be fitted by a linear function, which extrapolated to $N_p/N_s = 1$ gives the threshold value of the hole density $\delta_t$. If the concentration of holes is close but still smaller than $\delta_t$, most of the system is occupied by the FM phase, while the rest forms an AFM island (or islands). Finally, for concentrations larger than $\delta_t$ the whole system would be in a fully polarized state. However, the latter regime is probably not accessible by the present approach. In the Nagaoka regime, the Ising and isotropic $t$–$J$ models give the same results because the physics of the Nagaoka regime is determined by the competition between the magnetic and kinetic energies. However, as soon as the FM bubble covers the whole system other mechanisms come into play, e.g., a direct hole-hole interaction and/or interference of the carriers paths around loops. Fig. 10 shows $\delta_t$ as a function of $J$ (the point $\delta_t = 0$, $J = 0$ is a result of the Nagaoka theorem). The obtained square–root dependence between both quantities follows immediately from Eq. (11) and the proportionality $N_p \propto N$ shown in Fig. 9.

### A. Analytical approach for finite doping

We consider the FM polaron of size $N_p$ with $N$ doped holes that can be treated as spinless noninteracting fermions. The FM polaron is furthermore placed in the hole-depleted Néel spin background. We furthermore consider the limit of small hole-density that allows for quadratic expansion of the single particle kinetic energy:

$$E^{(1)}_\text{kin}(k) = -2(\cos k_x + \cos k_y) \sim -4 + k^2.$$  \hfill (16)

We obtain the kinetic energy of $N$ holes by integrating Eq. (16) up to $k_F = 2\sqrt{\pi N/N_p}$

$$E_\text{kin} = -4N + 2\pi N^2/N_p.$$ \hfill (17)

We proceed by writing the total energy $E(N)$ as:

$$E(N) = E_\text{kin} + E_\text{spin},$$

$$E(N) = -4N + 2\pi N^2/N_p + N_p J,$$ \hfill (18)

where the last term represents the magnetic energy of the FM polaron relative to the energy of the Néel state. After the minimization $\partial E/\partial N_p = 0$ we obtain

$$\frac{N_p}{N_s} = \sqrt{\frac{2\pi}{|J|}} \delta,$$ \hfill (19)

representing the ratio between the polaron size $N_p$ and the total size of the system $N_s$ as a function of hole doping $\delta$. The comparison of Eq. (19) with numerical data is shown in Fig. 9. From Eq. (19) we obtain as well the critical doping for the transition to the FM state

$$\delta_t = \sqrt{\frac{|J|}{2\pi}},$$ \hfill (20)

shown along the numerical results in Fig. 10. Notice, that Eq. (20) agrees with that derived within the semiclassical calculations of the 2D isotropic $t$–$J$ model, which suggest that at small hole concentration and rather weak AFM coupling the FM Nagaoka state becomes unstable towards a creation of an AFM bubble. This agreement is quite natural, since the spins are considered to be frozen in both the classical large-spin limit of the isotropic $t$–$J$ model and its full Ising version. Finally, we obtain the total energy of the system

$$E(N) = -4t \left(1 - \sqrt{\frac{\pi J}{2}}\right) N.$$ \hfill (21)

The comparison with numerical results is shown in Fig. 8. Here we have neglected the effects along the line, separating the FM polaron from the Néel spin background as well as the dependence of the kinetic energy on the shape of the bubble. As a results only the linear term in $E(N)$ is reproduced. Since the phase separation is determined by the nonlinear part of $E(N)$, these effects give rise to small, nevertheless important corrections. The former one is proportional to the length of the borderline ($\propto \sqrt{N}$) and it was the reason for the choice of the fitting function in Fig. 8.
FIG. 7: (Color online) Leftmost column: shapes of the Nagaoka polarons including from 2 to 5 holes. Filled circles indicate spin-up lattice sites and empty circles spin-down lattice sites. The rest of the panels show wave functions of the holes. In all cases $J=0.03$ was assumed.
VI. SUMMARY

The main difficulty in analyzing the $t$–$J$ model in the small–$J$ limit is that a large size of the lattice is required to correctly describe the dynamics of holes. This requirement significantly restricts the applicability of numerical approaches like the quantum MC or exact diagonalization method.

In the small–$J$ regime, however, the holes are confined in a FM polaron, so that the spin–flip processes are strongly reduced. This justifies the applicability of the Ising version of the $t$–$J$ model to study the small–$J$ limit of the original $t$–$J$ model.

For small but finite values of $J$, our results for one and two holes are in a good agreement with those obtained within the fully quantum approaches (DMRG, EDLFS). However, we are able to extend our calculations to the regimes of smaller $J$ and larger number of holes inaccessible by the former methods. We show that it is energetically favorable for the system to segregate into the FM hole–rich phase and hole–depleted AFM phase. The size (surface) of the FM bubble depends linearly on the number of holes while its dependence on $J$ is given by the square–root function. With increasing concentration of holes and/or with decreasing $J$ the size of the FM polaron increases and eventually for $\delta_t \simeq 0.44\sqrt{J}$ it occupies the whole lattice. Our numerical results thus suggest that Nagaoka state breaks down by forming an AFM bubble. This observation fully agrees with a conjecture discussed earlier within the isotropic $t$–$J$ model. We, however, expect that the results obtained for isotropic and Ising $t$–$J$ models start to deviate from each other when doping becomes larger that the threshold density $\delta_t$ even for $J \ll 1$.

A rather simple analytic treatment of the holes doped in the FM polaron that is furthermore placed in a Néel, hole-depleted spin background, leads to a good agreement with numerical data. Among other results, it provides a simple expression for the threshold density $\delta_t = \sqrt{J/2\pi}$. The theory reproduces only the linear dependence of the total energy on the number of holes and does not provide information on whether the system phase separates. Corrections (e.g., due to line contributions) are expected to give rise to a positive $\sqrt{N}$ term in the total energy, as obtained from the numerical data.
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