Phase separation in the large-spin t-J model

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We investigate the phase diagram of the two-dimensional t-J model using a recently developed technique that allows one to solve the mean-field model Hamiltonian with a variational calculation. The accuracy of our estimate is controlled by means of a small parameter $1/q$, analogous to the inverse spin magnitude $1/s$ employed in studying quantum spin systems. The mathematical aspects of the method and its connection with other large-spin approaches are discussed in detail. In the large-q limit the problem of strongly correlated electron systems turns into the minimization of a total-energy functional. We have performed this optimization numerically on a finite but large $L \times L$ lattice. For a single hole the static small-polaron solution is stable except for small values of J, where polarons of increasing sizes have lower energy. At finite doping we recover phase separation above a critical J and for any electron density, showing that the Emery *et al.* picture represents the semiclassical behavior of the t-J model. Quantum fluctuations are expected to be very important, especially in the small-J–small-doping region, where phase separation may also be suppressed.

I. INTRODUCTION

The discovery of high-temperature superconductors has renewed interest in the study of strongly interacting electron systems in one and two dimensions, because it is widely believed that the anomalous properties of such materials may be related to the strong Coulomb repulsion and to the low effective dimensionality.

One of the most interesting models which exactly incorporates the constraint of strong Coulomb repulsion is the well-known t-J model, which will be the main topic of the present paper. Several approximate techniques have been proposed so far to deal with this model Hamiltonian. We mention, for example, the self-consistent Born approximation,[1] the semiclassical approach,[2] and recently the limit of infinite dimensionality,[3] which have been developed for the one-hole case. In the general case of arbitrary density, the large-N expansion with slave-boson and the slave-fermion techniques[4] should also be mentioned, as well as the vast amount of numerical and variational works.[5] The results of all these different methods are quite controversial, especially concerning the question of the presence in the model of superconductivity and/or of marginal Fermi liquid behavior.

Quite recently, Emery, Kivelson, and Lin[6] tried to explain the full phase diagram of the model, basing their analysis both on a variational argument in the small-J region and on some numerical evidences emerging from a 4×4 lattice exact diagonalization. They speculated that *phase separation* should occur throughout the full phase diagram: The electron-system phase separates into a phase where the holes move in a fully polarized state and into an electron-rich phase characterized by a Néel antiferromagnetic spin order. Accordingly, phase separation occurs below some critical doping δ_c, where $\delta_c \to 0$ for $J \to 0$. Castellani *et al.*[7] then argued that superconductivity may occur close to the phase separation boundary. A numerical work by Ogata *et al.*[8] provided a complete determination of the one-dimensional phase diagram and evidenced this property in one dimension.

After the work of Emery, Kivelson, and Lin, Putikka, Luchini, and Rice[9] performed a systematic high-temperature expansion on the t-J model and found evidence that the separated phase should appear only for large values of J. Although this work is surely nonconclusive, they pointed out that there is not convincing evidence that the separated phase should be continuously connected through the whole phase diagram, because the small-J and large-J regions should behave in a very different way.

Because of the present controversy, we derive here a consistent mean-field calculation on the t-J model using a recently developed technique[10] allowing control of the accuracy of the mean-field estimate by means of a small parameter $1/q$, which is similar to the parameter $1/s$—the inverse spin magnitude—used in the spin-wave theory of quantum spin systems. This technique has the following advantages: (i) It conserves the symmetries of the t-J model Hamiltonian, (ii) takes exactly into account the constraint of no-double occupancy, and (iii) ensures that the classical estimate of the energy is *variational* for any value of q. In this way we generalize a very useful property known to hold for spin systems; i.e., the classical solution is independent of the spin magnitude and the corresponding energy is therefore variational.

With our mean-field approach we are able to reproduce the phase separation over the small- and large-J regions, supporting at the semiclassical level the picture of Emery, Kivelson, and Lin. We have made an intensive and systematic numerical work in order to calculate the true phase diagram at the mean-field level without imposing any *a priori* order parameter. At the end the phase diagram looks extremely simple, but unfortunately poor. However, our calculation represents only the first step towards a complete determination of the phase diagram. As standard in any semiclassical approach, the second step would be to include quantum fluctuations about the mean field. With the present technique corrections to the classical energy can be introduced systematically.

The paper is organized as follows: In Sec. II we review the graded Holstein-Primakoff map[10] for the graded algebra spl(2,1) and present the associated coherent states. These mathematical tools are developed starting from the observation that spl(2,1) is the algebra of the operators entering the strongly correlated electron systems and that it has a series of representation characterized by a parameter q analogous to the spin magnitude. The small parameter $1/q$ allows a systematic definition of distinct large-spin limits of the t-J model. In Sec. III we investigate the physical implications underlying the different generalizations of the model and show that previously proposed effective Hamiltonians, notably the Kane-Lee-Read[1] and the spinless fermion hopping Hamiltonians,[11] can be derived as particular cases of our approach. In Sec. IV we then derive the variational total-energy functional which solves our mean-field theory and present the results concerning the numerical investigation. Section V contains the conclusions.

II. spl(2,1) COHERENT STATES

The t-J model Hamiltonian[12] is defined by

$$H_{tJ} = t\sum_{ij,a}\Omega_{ij}\tilde{c}^{\dagger}_{ai}\tilde{c}_{aj} + \frac{J}{2}\sum_{ij}\Omega_{ij}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4}\hat{N}_i\hat{N}_j\right), \tag{2.1}$$

where $a = 1,2$ are spin-up and spin-down indices, respectively; Ω_{ij} is the adherence matrix with periodic boundary conditions connecting nearest-neighbor sites, i,j denote the lattice coordinates,

$$\tilde{c}_{1i} = (1 - c^{\dagger}_{2i}c_{2i})c_{1i}\ ,\quad \tilde{c}^{\dagger}_{1i} = c^{\dagger}_{1i}(1 - c^{\dagger}_{2i}c_{2i})\ ,$$
$$\tilde{c}_{2i} = (1 - c^{\dagger}_{1i}c_{1i})c_{2i}\ ,\quad \tilde{c}^{\dagger}_{2i} = c^{\dagger}_{2i}(1 - c^{\dagger}_{1i}c_{1i}) \tag{2.2a}$$

are hole creation-annihilation operators,

$$\hat{N}_i = (c^{\dagger}_{1i}c_{1i} + c^{\dagger}_{2i}c_{2i})\ ,\quad S_{3i} = \tfrac{1}{2}(c^{\dagger}_{1i}c_{1i} - c^{\dagger}_{2i}c_{2i})\ ,$$
$$S_{1i} = \frac{1}{2}(c^{\dagger}_{1i}c_{2i} + c^{\dagger}_{2i}c_{1i})\ ,\quad S_{2i} = \frac{1}{2i}(c^{\dagger}_{1i}c_{2i} - c^{\dagger}_{2i}c_{1i}) \tag{2.2b}$$

are charge and spin operators, where $c^{\dagger}_{1i}$, $c^{\dagger}_{2i}$ are the electron operators, and doubly occupied sites are excluded. The exchange constant is always positive: $J \geq 0$.

The 3×3 Hubbard matrices are defined by taking the expectation values of the operators (2.2) in the restricted single-site Hilbert space $|0_i\rangle$, $|1_i\rangle = c^{\dagger}_{1i}|0_i\rangle$, $|2_i\rangle = c^{\dagger}_{2i}|0_i\rangle$:

$$\chi_{ai} = \langle\alpha_i|\,\tilde{c}_{ai}\,|\beta_i\rangle\ ,\quad C_i = \langle\alpha_i|\,\hat{N}_i\,|\beta_i\rangle\ ,$$
$$\chi^a_i = \langle\alpha_i|\,\tilde{c}^{\dagger}_{ai}\,|\beta_i\rangle\ ,\quad \mathbf{Q}_i = \langle\alpha_i|\,\mathbf{S}_i\,|\beta_i\rangle\ ,\quad \alpha,\beta = 0,1,2\ . \tag{2.3}$$

The matrices χ^a_i and χ_{ai} are conjugate, i.e., $\chi^a_i = \chi^{\dagger}_{ai}$. However, for later convenience we prefer to use the notation with the raised index. The matrices (2.3) are useful because the constraint of no-double occupancy can be automatically taken into account by replacing in Eq. (2.1) the operators (2.2) with the corresponding matrices (2.3). Defining $Q_{0i} \equiv (I - \frac{1}{2}C_i)$, where I is the identity matrix, the Hubbard matrices (2.3) can be divided into odd (i.e., fermionic) generators χ_{ai}, χ^a_i and even (i.e., bosonic) generators $Q_{\mu i} = (Q_{0i}, \mathbf{Q}_i)$—which we collect in four-vectors—satisfying the commutation-anticommutation relations of the spl(2,1) graded algebra,[10,13]

$$[Q_{\mu i}, Q_{\nu j}] = \delta_{ij} i\epsilon_{0\mu\nu}{}^{\lambda}Q_{\lambda j}\ , \tag{2.4a}$$
$$[\chi^a_i, Q_{\mu j}] = \delta_{ij}\tfrac{1}{2}(\sigma_\mu)^a_b\chi^b_j\ , \tag{2.4b}$$
$$\{\chi_{ai}, \chi^b_j\} = \delta_{ij}(\sigma^\mu)^b_a Q_{\mu j}\ ,\quad \{\chi_{ai}, \chi_{bj}\} = 0\ , \tag{2.4c}$$

where the completely antisymmetric tensor is normalized by $\epsilon_{012}{}^3 = 1$, whereas the spin four-vector is built from the standard Pauli matrices as $(\sigma^\mu)^b_a \equiv (\delta_{ab}, \boldsymbol{\sigma}_{ab})$. The Greek four-vector indices are raised and lowered using the metric tensor $g_{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$, and a summation over repeated Lorentz and Latin (spinor) indices is understood. The generator Q_{0i} has to be introduced in order to close the spl(2,1) algebraic rules [Eqs. (2.4b) and (2.4c)]. For the time being our considerations will refer mostly to single-site quantities and to simplify the notation the site index will be dropped if not otherwise needed.

As explained in detail in Ref. 14, the several classes of irreducible representations of the spl(2,1) graded algebra are labeled by the eigenvalues of the operators Q_0, $\mathbf{Q}^2$, and Q_3, respectively denoted q_0, $q(q+1)$ (q is called isospin and is an integer or half-integer number), and q_3. The basis vectors are thus denoted with $|q_0, q, q_3\rangle$. Among them, those relevant for our investigation are the so-called atypical representations. They are characterized by a linear relation between q_0 and q and are thus identified only by the value of the isospin q, this being the parameter which we shall use analogously to the spin magnitude s in the standard spin-wave theory of the Heisenberg Hamiltonian. In each such atypical representation, of dimensionality $(4q+1)$, the basis vectors can be grouped into two multiplets of $(2q+1)$ and $2q$ states with quantum numbers

$$|q, q, q_3\rangle,\quad q_3 = -q, -q+1, \ldots, q, \tag{2.5a}$$
$$|q+\tfrac{1}{2}, q-\tfrac{1}{2}, q_3\rangle,\quad q_3 = -q+\tfrac{1}{2}, \ldots, q-\tfrac{1}{2}, \tag{2.5b}$$

which we assume as even and odd, respectively (the grading of the states is a pure matter of convention). The relative normalization of the two multiplets is not *a priori* fixed. For the isospin value $q = \frac{1}{2}$ the states (2.5) are the real spin-$\frac{1}{2}$ and hole (spin-0) states, respectively, and the matrices defining the representation turn in the 3×3 Hubbard matrices. Thus the operators (2.2) entering the t-J model belong to the fundamental $q = \frac{1}{2}$ atypical representation of spl(2,1). According to Eqs. (2.5), models of strongly correlated electron systems can be generalized in a natural way by enlarging the dimensionality of the spl(2,1) representation. In particular we are naturally lead to identify the multiplet (2.5a) as the generalized spin state and the multiplet (2.5b) as the generalized hole state. The different value of q_0 between the two multiplets is related to the grading. Defining the "fermion number operator" $F = 2Q_0 - 2qI$, where I is the unit matrix of the q representation, then the spin multiplet (2.5a) has $F = 0$ and the hole multiplet (2.5b) has $F = 1$. Thus for a many-particle system the conservation of the number of particles can be rewritten as the conservation of the fermion number,

$$\sum_{i=1}^{N} F_i = \sum_{i=1}^{N}(2Q_{0i} - 2qI) = N_h = N - N_{\text{el}}, \qquad (2.6)$$

where N_{el} is the number of electrons, N is the number of sites, and thus N_h is the number of holes.

Assuming the maximal isospin state as the reference vacuum, $|0\rangle \equiv |q,q,q\rangle$ (not to be confused with the electronic empty state), and introducing a canonical boson a and a canonical spinless fermion c, then the $(4q+1)$-dimensional Hilbert space spanned by the states (2.5) can be put into correspondence with the Fock space generated by the states $|B,n\rangle = (a^\dagger)^n|0\rangle$ [corresponding to Eq. (2.5a)], and $|F,n\rangle = c^\dagger(a^\dagger)^n|0\rangle$ [corresponding to Eq. (2.5b), with $|F,0\rangle = |q+\frac{1}{2}, q-\frac{1}{2}, q-\frac{1}{2}\rangle$], satisfying the operatorial relation $a^\dagger a + c^\dagger c \leq 2q$.

In this basis, the generators (2.4) can be represented as[10]

$$\begin{aligned} &Q_0 = q + \tfrac{1}{2}c^\dagger c\,, \quad \chi_1 = c^\dagger\sqrt{2q - a^\dagger a - c^\dagger c}\,, \\ &Q_3 = q - a^\dagger a - \tfrac{1}{2}c^\dagger c\,, \quad \chi^1 = \sqrt{2q - a^\dagger a - c^\dagger c}\; c\,, \\ &Q_+ = \sqrt{2q - a^\dagger a - c^\dagger c}\; a\,, \quad \chi_2 = c^\dagger a\,, \\ &Q_- = a^\dagger\sqrt{2q - a^\dagger a - c^\dagger c}\,, \quad \chi^2 = a^\dagger c\,, \end{aligned} \qquad (2.7)$$

where $Q_\pm = Q_1 \pm iQ_2$. Note that the representation of χ_1 (and χ^1) can be simplified; i.e., we have $\chi_1 = c^\dagger\sqrt{2q - a^\dagger a}$. The symmetric notation (2.7) is useful to check that Eqs. (2.7) satisfy to Eqs. (2.4). These equations represent the generalization to spl(2,1) of the usual Holstein-Primakoff (HP) transformation[15] for su(2) and in this respect are similar to those of the Swinger-bosons–slave-fermion representation.[16] Using the realization (2.7) of the generator Q_0, the conservation law (2.6) becomes the conservation of the spinless fermion number operator; $\hat{N}_h \equiv \sum_i c_i^\dagger c_i = N_h$, so that at half-filling (i.e., $N_h = 0$) Eqs. (2.7) reduce to the standard su(2) HP transformation

$$\begin{aligned} &Q_3 = s - a^\dagger a\,, \\ &Q_+ = \sqrt{2s - a^\dagger a}\; a\,, \\ &Q_- = a^\dagger\sqrt{2s - a^\dagger a}\,, \end{aligned} \qquad (2.8)$$

where $a^\dagger a \leq 2s$ (using the standard symbol s instead of q), in agreement with the result that at half-filling the t-J model becomes the antiferromagnetic (AF) Heisenberg model.

As for spin systems, we wish to describe spin configurations classically. To this aim we need the transformations $(Q_\mu, \chi_a) \to (P_\mu, X_a)$ of the generators which preserve the spl(2,1) algebra. This can be conveniently done by choosing the original fermionic representation (2.2) of the $q = \frac{1}{2}$ generators (2.3), and then considering the most general transformation of the electron operators which preserves the canonical commutation relations (2.4) as well as the constraint of no-double occupancy. Simple algebra shows that the odd generators transform like su(2) operators in the fundamental representation:

$$\begin{aligned} &X_1 = e^{i\gamma}e^{-i\frac{\phi}{2}}\left(\cos\frac{\theta}{2}e^{i\frac{\psi}{2}}\chi_1 - \sin\frac{\theta}{2}e^{-i\frac{\psi}{2}}\chi_2\right), \\ &X_2 = e^{i\gamma}e^{i\frac{\phi}{2}}\left(\sin\frac{\theta}{2}e^{i\frac{\psi}{2}}\chi_1 + \cos\frac{\theta}{2}e^{-i\frac{\psi}{2}}\chi_2\right), \\ &X^1 = X_1^\dagger\,, \quad X^2 = X_2^\dagger\,, \end{aligned} \qquad (2.9)$$

whereas the even generators transform as

$$P_0 = Q_0\,, \quad P_k = R_{km}Q_m, \qquad (2.10)$$

where R_{km} is the SO(3) rotation matrix, whose explicit realization can be easily derived by means of the anticommutation rule (2.4c). By retaining only the leading-order terms of the HP transformation (2.7) we have $Q_0 = Q_3 \to q$, $Q_\pm \to 0$, $\chi_1 \to \sqrt{2q}\,c^\dagger$, $\chi_2 \to 0$, so that in the large-q limit the rotated even generators (2.10) become classical c-numbers,

$$\begin{aligned} &P_\mu \to q(1,\mathbf{n}) \equiv p_\mu\,, \\ &\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \end{aligned} \qquad (2.11)$$

and the rotated odd generators (2.9) become proportional to the spinless fermion operator,

$$\begin{aligned} &X_1 \to \sqrt{2q}\,e^{i\omega}e^{-i\frac{\phi}{2}}\cos\left(\frac{\theta}{2}\right)c^\dagger\,, \quad X^1 = X_1^\dagger, \\ &X_2 \to \sqrt{2q}\,e^{i\omega}e^{i\frac{\phi}{2}}\sin\left(\frac{\theta}{2}\right)c^\dagger\,, \quad X^2 = X_2^\dagger\,, \end{aligned} \qquad (2.12)$$

where we have set $\omega = \gamma + \psi/2$.

In the previous equations θ and ϕ are the physical angles which parametrize the classical spin configuration [see Eq. (2.11)]. Instead, the third Euler angle ψ and the global fermionic phase γ are unessential. In fact, ψ can always be eliminated by redefining $\tilde{Q}_\pm \equiv e^{\mp i\psi}Q_\pm$, $\tilde{\chi}_2 \equiv e^{-i\psi/2}\chi_2$, $\tilde{\chi}_1 \equiv e^{i\psi/2}\chi_1$, and γ can be arbitrarily fixed by changing the relative normalization of the two multiplets (2.5).

Similarly to spin models, we can give to Eqs. (2.11) and (2.12) a quantum-mechanical meaning by introducing the even coherent state $|\Omega_b\rangle$ of the generalized spin multiplet (2.5a) and the odd coherent state $|\Omega_f\rangle$ of the generalized hole multiplet (2.5b):

$$|\Omega_b\rangle = \left(\cos\frac{\theta}{2}\right)^{2q}\exp\left(\tan\frac{\theta}{2}e^{i\phi}Q_-\right)|B,0\rangle\,, \qquad (2.13a)$$

$$|\Omega_f\rangle = \left(\cos\frac{\theta}{2}\right)^{2q-1}\exp\left(\tan\frac{\theta}{2}e^{i\phi}Q_-\right)|F,0\rangle\,. \qquad (2.13b)$$

The states (2.13) are orthonormal and by generalizing standard results[17] on su(2) coherent states we find

$$\langle\Omega_b|Q_\mu|\Omega_b\rangle = q(1,\mathbf{n}) = p_\mu, \quad \langle\Omega_b|Q_\mu|\Omega_f\rangle = 0, \tag{2.14a}$$

$$\langle\Omega_f|Q_\mu|\Omega_f\rangle = (q+\tfrac{1}{2},(q-\tfrac{1}{2})\mathbf{n}) = p'_\mu. \tag{2.14b}$$

As for the su(2) coherent states, the classical c-numbers (2.11) are equal to the expectation value of the even generators between the even coherent states. The spin expectation value $\langle\Omega_f|\mathbf{Q}|\Omega_f\rangle$ is in general finite and it is zero only for the value $q=\frac{1}{2}$, an obvious consequence of the fact that the generalized hole is actually a spin-$(q-\frac{1}{2})$ multiplet. Concerning the odd generators, it is easily checked that

$$\begin{aligned}
\chi_1|\Omega_b\rangle &= \sqrt{2q}\, e^{i(\omega-\frac{\phi}{2})}\cos\left(\frac{\theta}{2}\right)|\Omega_f\rangle\,,\\
\chi^1|\Omega_f\rangle &= \sqrt{2q}\, e^{-i(\omega-\frac{\phi}{2})}\cos\left(\frac{\theta}{2}\right)|\Omega_b\rangle\,,\\
\chi_2|\Omega_b\rangle &= \sqrt{2q}\, e^{i(\omega+\frac{\phi}{2})}\sin\left(\frac{\theta}{2}\right)|\Omega_f\rangle\,,\\
\chi^2|\Omega_f\rangle &= \sqrt{2q}\, e^{-i(\omega+\frac{\phi}{2})}\sin\left(\frac{\theta}{2}\right)|\Omega_b\rangle\,,\\
\chi_a|\Omega_f\rangle &= 0\,,\quad \chi^a|\Omega_b\rangle = 0,
\end{aligned} \tag{2.15}$$

where we have fixed the relative normalization of the states (2.5) by using the phase convention $\chi_1|B,0\rangle = \sqrt{2q}\,e^{i(\omega-\frac{\phi}{2})}|F,0\rangle$. From Eq. (2.15) it follows that the combination of odd generators,

$$\chi^\dagger = \frac{e^{-i\omega}}{\sqrt{2q}}\left[e^{i\frac{\phi}{2}}\cos\left(\frac{\theta}{2}\right)\chi_1 + e^{-i\frac{\phi}{2}}\sin\left(\frac{\theta}{2}\right)\chi_2\right], \tag{2.16}$$

creates the odd coherent state out of the even one, whereas the conjugate operator annihilates it:

$$\chi^\dagger|\Omega_b\rangle = |\Omega_f\rangle,\quad \chi|\Omega_b\rangle = 0. \tag{2.17a}$$

We also have

$$\chi|\Omega_f\rangle = |\Omega_b\rangle,\quad \chi^\dagger|\Omega_f\rangle = 0. \tag{2.17b}$$

The relations (2.17a) show that $\chi^\dagger$ and χ are the q-generalized hole creation and annihilation operators, respectively, and Eq. (2.17b) acquires the meaning of the particle-hole transformation. Note that $\chi^\dagger$, χ are not spinless fermion operators, because for a generic q representation their anticommutator (restoring the notation with the site index) is $\{\chi_i^\dagger,\chi_j\} = \delta_{ij}\frac{1}{2q}(Q_{0j}+\mathbf{Q}_j\mathbf{n}_j)$. However, this means that the identity

$$\langle\mathbf{\Omega}|\{\chi_i^\dagger,\chi_j\}|\mathbf{\Omega}\rangle = \delta_{ij} \tag{2.18}$$

is satisfied, so that $\chi_i^\dagger$, χ_i act like spinless fermion operators when bracketed between any tensor product of even and/or odd coherent states $|\mathbf{\Omega}\rangle = \bigotimes|\Omega_{\alpha i}\rangle$ $(\alpha=b,f)$.

III. LARGE-SPIN LIMIT

Here and in the following we shall refer to the *large-spin limit* whenever the single-site Hilbert space of a strongly correlated electron system is enlarged by assuming a spin-q multiplet as the spin state and a spin-$(q-\frac{1}{2})$ multiplet as the hole state, and then one lets $q\to\infty$. To develop the coherent states for spl(2,1) we have constantly used the operator Q_{0i}, because this is the generator by which the spl(2,1) algebraic rules (2.4) can be closed and thus the spl(2,1) representation theory (2.5) applied. However, in the t-J model Hamiltonian there enters the charge operator $\hat{N}_i$, and we have to define its large-q generalization. As a matter of fact, here we are faced with the more general problem of how to generalize the t-J model itself, because the large-q generalization of the charge and spin operators has a certain amount of arbitrariness. On the one hand, to perform the large-spin limit of the t-J model we may straightforwardly use the linear generalization of the operators (2.2). This amounts to replacing in Eq. (2.1),

$$\tilde{c}_{ai}\to\chi_{ai},\quad \mathbf{S}_i\to\mathbf{Q}_i,\quad \hat{N}_i\to C_i = 2(2qI-Q_{0i}), \tag{3.1}$$

where $(\chi_{ai},Q_{\mu i})$ have now arbitrary isospin magnitude q. The last modification generalizes the relation $C_i = 2(I-Q_{0i})$ of the original $q=\frac{1}{2}$ theory. We have $C_i|\Omega_{bi}\rangle = 2q|\Omega_{bi}\rangle$ and $C_i|\Omega_{fi}\rangle = (2q-1)|\Omega_{fi}\rangle$, which means that the spin and hole states (2.5) have generalized spin—differing by half-unit—as well as generalized electric charge—differing by one unit.

On the other hand, for the $q=\frac{1}{2}$ fundamental representation, and only in this case, the 3×3 Hubbard matrices (2.3) satisfy

$$\begin{aligned}
C_i &= (\chi_i^1\chi_{1i}+\chi_i^2\chi_{2i}),\quad Q_{3i} = \tfrac{1}{2}(\chi_i^1\chi_{1i}-\chi_i^2\chi_{2i}),\\
Q_{1i} &= \frac{1}{2}(\chi_i^1\chi_{2i}+\chi_i^2\chi_{1i}),\quad Q_{2i} = \frac{1}{2i}(\chi_i^1\chi_{2i}-\chi_i^2\chi_{1i}),
\end{aligned} \tag{3.2}$$

a consequence of the fact that whether the constraint of no-double occupancy is enforced, the charge and spin operators (2.2b) are unchanged if we substitute the electron operators with the corresponding hole operators (2.2a). According to the previous equation, we may think of the charge and spin operators (2.2b) as composite operators of the odd generators for any value of q, so that we may also define the large-spin limit of Eq. (2.1) by means of the replacement

$$\tilde{c}_{ai}\to\chi_{ai},\quad \mathbf{S}_i\to\boldsymbol{\mathcal{Q}}_i = \tfrac{1}{2}\chi_i^a\boldsymbol{\sigma}_{ab}\chi_{bi},\quad \hat{N}_i\to\mathcal{C}_i = \chi_i^a\chi_{ai}, \tag{3.3}$$

where χ_{ai}, χ_i^a have now arbitrary isospin magnitude q. The present generalization amounts to consider Eq. (2.1) as a model of interacting holes and to preserve this dynamics for any value of the hole isospin. For any $q\neq\frac{1}{2}$, Eqs. (3.1) and (3.3) are not equivalent and in our analysis we shall investigate the physical implications underlying the two choices.

The simplest generalization is obtained by choosing the linear realization (3.1). Using the arbitrarily rotated frame (P_μ, X_a) [Eqs. (2.10) and (2.9)], upon the substitution (3.1) the generalized t-J model Hamiltonian becomes

$$H_{tJ}^{(q)} \equiv t\sum_{ij,a}\Omega_{ij}X_i^aX_{aj} + \frac{J}{2}\sum_{ij}\Omega_{ij}\left(\mathbf{P}_i\mathbf{P}_j - \frac{1}{4}C_iC_j\right)$$
$$= t\sum_{ij,a}\Omega_{ij}X_i^aX_{aj} - \frac{J}{2}\sum_{ij,\mu\nu}\Omega_{ij}g^{\mu\nu}P_{\mu i}P_{\nu j}$$
$$+4qJN_h, \qquad (3.4)$$

where in the last identity we have applied the conservation law (2.6). Similarly to spin systems, using the linear generalization we preserve all the symmetries of the original model. Apart from a trivial constant, Eq. (3.4) is bilinear in the spl(2,1) generators, so that $J = 2t$ remains the "supersymmetric point"[18] for any value of the isospin q. Replacing the HP map (2.7) in Eq. (3.4), in the $q \to \infty$ limit the potential energy becomes dominant, so that the large-spin limit of Eq. (3.4) is given by the classical Heisenberg model

$$H_{tJ}^{(q)} \to H_H^{\rm class} = \frac{Jq^2}{2}\sum_{ij}\Omega_{ij}\left(\mathbf{n}_i\mathbf{n}_j - 1\right). \qquad (3.5)$$

Thus for any electron density $\rho = N_{\rm el}/N$ the mean-field solution is always the Néel spin configuration. We can easily understand this result noting that in the large-q limit the expectation values [Eqs. (2.14a) and (2.14b)] are equal:

$$\lim_{q\to\infty}\frac{p_{\mu i}}{q} = \lim_{q\to\infty}\frac{p'_{\mu i}}{q} = (1, \mathbf{n}_i). \qquad (3.6)$$

As a consequence in the large-q limit we still have two distinct states $|\Omega_{bi}\rangle$ and $|\Omega_{fi}\rangle$ differing by the fermion number F_i; however, their spin and charge become equal. Hence the mean-field theory turns in the AF spin Hamiltonian, independently from the density. Thus in the large-spin limit we preserve all the symmetries, but we miss the following important property of the exact model (2.1): If the hole is localized on site i_0, the four bonds $J\Omega_{i_0j}$ do not contribute to the energy (we shall refer to this property as the "dynamics of the missing bonds"). This is a peculiar behavior of the present large-spin limit. However, all the developments are mathematically well defined and the expansion in fluctuations about the AF mean-field solution can be performed straightforwardly. We divide the lattice into two sublattices, and in Eqs. (2.9) and (2.10) set $\theta = \phi = \psi = \gamma = 0$ on one sublattice and $\theta = \psi = \pi$, $\phi = 0$, $\gamma = -\pi/2$ on the other one. Then the replacement in Eq. (3.4) of the HP realization (2.7) expanded in powers of $1/q$ gives the effective Hamiltonian

$$H^{\rm KLR} = E_0 + \frac{qJ}{2}\sum_{ij}\Omega_{ij}\left(a_i^\dagger a_i + a_j^\dagger a_j + a_i^\dagger a_j^\dagger + a_ia_j\right)$$
$$-\sqrt{2q}\,t\sum_{ij}\Omega_{ij}c_i^\dagger c_j(a_j^\dagger + a_i) + \cdots \qquad (3.7)$$

to describe fluctuations, where

$$E_0 = -4NJq^2 + 4Jq\sum_i c_i^\dagger c_i \qquad (3.8)$$

is the classical energy of the pure antiferromagnet plus a quantum contribution which shifts the chemical potential of the spinless fermions. In Eq. (3.7) we have displayed only the first few terms of the systematic expansion. They give exactly the Hamiltonian proposed and applied by Kane, Lee, and Read[1] (KLR) to describe the propagation of a single hole in a quantum antiferromagnet. In their approach the bosonic term and the three-body term—the latter responsible for the hole propagation through spin-wave emission and absorbtion—are treated on equal footing. This assumption corresponds to scaling t by a factor $\sqrt{2q}$ and then define the large-spin limit keeping fixed the renormalized hopping parameter $t_0 = t/\sqrt{2q}$. Equation (3.7) is well defined for any density and from Eq. (3.8) we see that in the large-spin limit (3.1) the dynamics of the missing bonds is present only when quantum fluctuations are taken into account. In particular setting $q = \frac{1}{2}$, we have $E_0 = -J(2N - 4N_h)/2$, which is the energy of the classical antiferromagnet with N_h delocalized holes.

The dynamics of the missing bonds is the essential feature of the t-J model to understand phase separation in cuprate superconductors, and it is completely not accounted for by the large-spin limit (3.1). This property can be preserved if we resort to the nonlinear generalization (3.3). All our considerations are simplified by introducing the projector onto the even sector:

$$\Gamma_i = (2q+1)I - 2Q_{0i}, \quad \Gamma_i|\Omega_{bi}\rangle = |\Omega_{bi}\rangle, \quad \Gamma_i|\Omega_{fi}\rangle = 0. \qquad (3.9)$$

Employing the HP transformation (2.7), it is easily shown that the even operators $(\mathcal{C}_i, \boldsymbol{\mathcal{Q}}_i)$ of the set (3.3) are related to the operators $(C_i, \mathbf{Q}_i)$ in Eq. (3.1) via the projector Γ_i:

$$\mathcal{C}_i = \Gamma_i^\dagger C_i\Gamma_i, \quad \boldsymbol{\mathcal{Q}}_i = \Gamma_i^\dagger \mathbf{Q}_i\Gamma_i. \qquad (3.10)$$

We collect the generalized charge and spin operators (3.3) in the four-vector $\mathcal{Q}_{\mu i} = \Gamma_i^\dagger Q_{\mu i}\Gamma_i$ (note that we have the relation $\mathcal{C}_i = \Gamma_i^\dagger C_i\Gamma_i = 2\mathcal{Q}_{0i}$). Applying Eqs. (3.9) and (3.10) we then have

$$\langle\Omega_{bi}|\mathcal{Q}_{\mu i}|\Omega_{bi}\rangle = p_{\mu i}, \quad \langle\Omega_{fi}|\mathcal{Q}_{\mu i}|\Omega_{fi}\rangle = 0. \qquad (3.11)$$

An independent check of Eq. (3.11) can be obtained by using the definition (3.3) and the rules (2.15). Since the projector (3.9) commutes with the even generators $Q_{\mu i}$ it is easily proved that the su(2)×u(1) even subalgebra is preserved,

$$[\mathcal{Q}_{\mu i}, \mathcal{Q}_{\nu j}] = i\delta_{ij}\epsilon_{0\mu\nu}{}^{\lambda}\mathcal{Q}_{\lambda j}, \qquad (3.12a)$$

so that the operators (3.10) under the rotation (2.9) of the odd generators, $\chi_{ai} \to X_{ai}$, are $(\mathcal{P}_{\mu i}, X_{ai})$, where

$$\mathcal{P}_{0i} = \mathcal{Q}_{0i} = \tfrac{1}{2}\mathcal{C}_{0i}, \quad \mathcal{P}_{ki} = X_i^a\sigma_{ab}^kX_{bi} = R_{km}\mathcal{Q}_{mi}, \qquad (3.12b)$$

R_{km} being the rotation matrix in Eq. (2.10). Upon the substitution (3.3) the generalized t-J model Hamiltonian in the rotated frame (3.12b) eventually becomes

$$H^{(q)}_{[X,\mathcal{P}]} = t\sum_{ij,a}\Omega_{ij}X^a_i X_{aj} +\frac{1}{2}\frac{J_0}{2q}\sum_{ij}\Omega_{ij}\left(\mathcal{P}_i\mathcal{P}_j - \frac{1}{4}\mathcal{C}_i\mathcal{C}_j\right). \quad (3.13)$$

Here we have defined the model keeping fixed the rescaled exchange constant $J_0 = 2qJ$, to weigh on equal footing the kinetic and potential energy contributions (we explicitly display the dependence of $H^{(q)}_{[X,\mathcal{P}]}$ on the operators for later convenience).

For arbitrary values of q we lose supersymmetry at the $J = 2t$ point because the set of operators $(\mathcal{Q}_{\mu i}, \chi_{ai})$ forms a representation of spl(2,1) only for $q = \frac{1}{2}$. However, because of Eqs. (3.12), the model (3.13) remains rotationally invariant and, thanks to Eq. (3.11), the dynamics of the missing bonds is now present for any value of the isospin q. Thus Eq. (3.13) has all the relevant properties of the t-J model we are interested in and we consider it as a physically sensible generalization.

In the canonical basis the operators (3.10) are given by the expressions

$$\begin{aligned}
&\mathcal{C}_i = 2qc_ic_i^\dagger, \quad \chi_{1i} = c_i^\dagger\sqrt{2q - a_i^\dagger a_i},\\
&\mathcal{Q}_{3i} = c_ic_i^\dagger(q - a_i^\dagger a_i), \quad \chi_i^1 = \sqrt{2q - a_i^\dagger a_i}\; c_i,\\
&\mathcal{Q}_{+i} = c_ic_i^\dagger\sqrt{2q - a_i^\dagger a_i}\; a_i, \quad \chi_{2i} = c_i^\dagger a_i,\\
&\mathcal{Q}_{-i} = c_ic_i^\dagger a_i^\dagger\sqrt{2q - a_i^\dagger a_i}, \quad \chi_i^2 = a_i^\dagger c_i.
\end{aligned} \quad (3.14)$$

Expanding in powers of $1/q$ the previous realizations, the large-spin limit of Eq. (3.13) turns in an interacting spinless fermion Hamiltonian embedded in a classical spin background,

$$H^{(q)}_{[X,\mathcal{P}]} \to H^{\rm eff}_{tJ} = -2qt\sum_{ij}\Omega_{ij}\langle\Omega_{bi}|\Omega_{bj}\rangle^{\frac{1}{2q}}c_i^\dagger c_j + \frac{qJ_0}{4}\sum_{ij}\Omega_{ij}\left(\mathbf{n}_i\mathbf{n}_j - 1\right)(1 - c_i^\dagger c_i)(1 - c_j^\dagger c_j), \quad (3.15)$$

where the overlap between even coherent states is

$$\langle\Omega_{bi}|\Omega_{bj}\rangle = \left(\cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2} + e^{-i(\phi_i-\phi_j)}\sin\frac{\theta_i}{2}\sin\frac{\theta_j}{2}\right)^{2q} \quad (3.16)$$

[so that the factor $\langle\Omega_{bi}|\Omega_{bj}\rangle^{1/(2q)}$ in Eq. (3.15) is q independent], and we have chosen the relative normalization of the multiplets (2.5) such that $\omega_i - \phi_i/2 = 0$.

A relevant feature of the effective Hamiltonian Eq. (3.15) is that it gives a variational estimate of the ground-state energy. Any further inclusion of $1/q$ fluctuations can only improve the estimate, and this is a remarkable property that in our approach is naturally preserved. To show this property, we consider the model (3.13) in the original frame, namely, with the operators $(\mathcal{P}_\mu, X_a)$ directly replaced by $(\mathcal{Q}_\mu, \chi_a)$, and denote it with $H^{(q)}_{[\chi,\mathcal{Q}]}$. According to Eqs. (2.15) and (2.16) and to the generalization (3.3) of the charge and spin operators (2.2b) the action of the Hamiltonian $H^{(q)}_{[\chi,\mathcal{Q}]}$ over the state

$$|\Psi^{(q)}\rangle = \prod_{l=1}^{N_h}\left(\sum_{i=1}^{N}\psi_l(i)\chi_i^\dagger\right)|\mathbf{\Omega}\rangle \quad (3.17)$$

is exactly given by the action of the effective spinless fermion Hamiltonian (3.15) over the free particle state $|\Psi\rangle$ obtained by replacing in Eq. (3.17) the operators $\chi_i^\dagger$ with spinless fermion operators $c_i^\dagger$ and the boson state $|\mathbf{\Omega}\rangle$ with the vacuum state $|0\rangle$ of the spinless fermion representation. Here $|\mathbf{\Omega}\rangle = \bigotimes|\Omega_{bi}\rangle$ is the tensor product of even coherent states and $\psi_l(i)$ are N_h complex and orthonormal orbitals ($l = 1, 2, ..., N_h$ in a d-dimensional hypercubic lattice $L^d = N$).

As a consequence, any variational estimate $\mathcal{E} = \langle\Psi|H^{\rm eff}_{tJ}|\Psi\rangle$ of the ground-state energy of the spinless fermion Hamiltonian (3.15) is also a variational estimate of the ground-state energy of the generalized t-J model (3.13). Moreover, simple algebra shows the notable identity

$$\mathcal{E} = \langle\Psi^{(q)}|H^{(q)}_{[\chi,\mathcal{Q}]}|\Psi^{(q)}\rangle = 2q\,\langle\Psi^{(\frac{1}{2})}|H_{tJ}|\Psi^{(\frac{1}{2})}\rangle, \quad (3.18)$$

where H_{tJ} is the exact $q = \frac{1}{2}$ model (2.1). The factor $2q$ simply rescales the unit of energy and this ensures that no spurious phase transitions as a function of q are present in connecting the large-spin "classical" solution $\mathcal{E}$ to the variational estimate of the exact model. For the time being we thus set $2q = 1$.

IV. LARGE-SPIN MEAN FIELD

Despite the notable simplification given by the disappearance of the constraint of double occupancy, Eq. (3.15) is still a difficult problem to solve because the spinless fermions interact via a four-body term. For the infinite-U Hubbard model, i.e., when $J = 0$, and for the case of a single hole the interaction term does not play any role. Thus in the large-q limit we end up with the study of a free Hamiltonian with a complicated site-dependent hopping, which can be easily solved numerically on a finite—but large—lattice, as we shall discuss. For low doping the Hartree-Fock factorization (3.17) is expected to be a good approximation since few holes can rarely interact. We extended the Hartree-Fock solution to the full phase diagram of the Hamiltonian (3.15). Although this is not completely justified, the interaction between spinless fermions should not drastically affect the mean-field phase diagram, since for example it is known that the Hartree-Fock solution is exact in $d \to \infty$ for a gas of interacting spinless fermions.[3]

Thanks to Eq. (3.18) it is possible to apply Wick's theorem and the classical energy on a given arbitrary state reads

$$\mathcal{E} = \sum_{ij} \Omega_{ij} \Bigg[-t\langle \Omega_{bi}|\Omega_{bj}\rangle g_{i,j} - \frac{J}{8}(\mathbf{n}_i\mathbf{n}_j - 1)(g_{i,i} + g_{j,j} - g_{i,i}g_{j,j} + g_{i,j}g_{j,i} - 1)\Bigg], \tag{4.1}$$

where $g_{i,j} = \sum_{l=1}^{N_h} \psi_l^*(i)\psi_l(j)$.

The classical energy is therefore a function of the $2N$ spin angles θ_i, ϕ_i and of the $N_h \times N$ complex variables defining the wave function (3.17). The lowest possible energy $\mathcal{E}_0$ as a function of all the $2N\times(1+N_h)$ real variables represents a variational classical estimate of the ground-state energy. We solved this optimization problem on a square lattice numerically, following a scheme which is similar to the one introduced by Car and Parrinello[19] for the electronic structure problem, i.e., for the simulation of the *slow* dynamics of the ions interacting via a self-consistent potential generated by the electronic *fast* degrees of freedom. This approach can be extended to our case because the isospin q behaves as an adiabatic parameter: in the $q \to \infty$ limit the spl(2,1) even generators (2.7) ("slow variables") become classical objects, so that Eq. (3.13) describes the dynamics of the odd and projection operators (2.7) and (3.9) ("fast variables") in the background of the former. Thus the electronic degrees of freedom have a much faster dynamic of the spin angles, which in this case play indeed the role of the ionic coordinates.

In order to minimize the numerical effort we first move the electronic degrees of freedom at a fixed spin configuration and then the spin angles without changing the electronic degrees of freedom. At each step we do not require a fully converged Hartree-Fock solution of the electronic part, but we make a fixed number of steepest-descent steps, followed by a Graham-Schmidt orthogonalization of the orbitals to achieve numerical stability. After many spin moves ($\approx$10 000) we get a fully self-consistent solution of the problem up to computer machine accuracy. The solution found with the previously described iterative scheme may not coincide with the absolute minimum—the classical ground state. The true minimum can be identified on a reasonable ground by resorting to symmetry considerations or by performing several simulations with different random initializations.

For $J = 0$ the mean-field Hamiltonian (3.15) becomes the free spinless fermion hopping Hamiltonian

$$H_t^{\text{eff}} = -t \sum_{ij} \Omega_{ij} \langle \Omega_{bi}|\Omega_{bj}\rangle c_i^\dagger c_j, \tag{4.2}$$

which has been phenomenologically introduced[11] to study the instability of the Nagaoka state—i.e., the free particle state with maximum allowed spin and lowest kinetic energy—in the infinite-U Hubbard model. The Nagaoka theorem[20] states that it is the exact ground state of the model in the one-hole case. Writing the coherent state overlap in the form[17]

$$\langle \Omega_{bi}|\Omega_{bj}\rangle = \sqrt{\frac{1+\mathbf{n}_i\cdot\mathbf{n}_j}{2}}\, e^{iA_{ij}}, \tag{4.3}$$

where A_{ij} is the solid angle subtended by the vectors $\mathbf{n}_i$, $\mathbf{n}_j$, and a reference fixed one $\mathbf{n}_0$, it has been conjectured that for more than one hole a nonfully polarized spin background may have better energy than the Nagaoka state, because the gain in magnetic energy due to the nonzero flux of A_{ij} could overwhelm the narrowing of the effective bandwidth $t\Omega_{ij} \to t\Omega_{ij}\sqrt{(1+\mathbf{n}_i\mathbf{n}_j)/2}$. In this case we have performed over 10 000 fully converged minimizations on a 10×10 and a 16×16 lattice and for arbitrary density. We initialize randomly the spins angles and set the orbitals $\psi_l(i)$ at the corresponding Hartree-Fock solution of the spinless fermion Hamiltonian with the chosen random spin configuration. In all the minimizations we have *never* found a solution with corresponding energy lower than the "Nagaoka energy." Most of the runs converge to the fully polarized solution. Only a few remain trapped into a local minimum of the classical energy. A particularly interesting case is at doping $\delta = N_h/N = 1/2$. In this case we have indeed found a stable planar solution with $\phi_i = 0$ and $\theta_i = \frac{2\pi}{L} i_x$, where $i_x = 0, 1, \ldots, L-1$ are the lattice coordinates along the x axis. This minimum configuration is similar to the one proposed by Doucqt and Wen for few holes.[11] However, we have found that this kind of state is always unstable except for this particular doping $\delta = 1/2$, and its energy is only degenerate with the Nagaoka energy. For large L this state tends (locally) to the Nagaoka state and leads in fact to the same correlation functions. Contrary to the Nagaoka state, this planar solution is not an exact eigenstate of the infinite-U Hubbard model. This fact represents a very simple proof that the Nagaoka state is not the true ground state at $\delta = 1/2$. Although our result about the stability of the Nagaoka state is based on a numerical optimization problem which is never completely reliable, we at least may argue that there is no evidence of any exotic spiral, flux, or chiral phase in the t-J model for $J = 0$ at the mean-field level.

For $J \neq 0$ we consider first the interesting case when only one hole is present. A recent reason of debate is whether the spiral mean-field solution of Shraiman and Siggia[2] has lower or higher energy compared to the polaronic solutions (see Fig. 1). As we have anticipated, also in this case we are left with the study of a free Hamiltonian with a complicated site-dependent hopping, to be adjusted as to minimize Eq. (4.1). The results of our numerical investigation confirm that the polarons are the lowest-energy configurations of the large-spin limit of the t-J model. The small-polaron solution, also called the five-site polaron [the hole is trapped in a given site and its nearest neighbors, see Fig. 1(a)], is stable for $J/t > 0.243$. For smaller J/t the size ξ of the polaron is gradually increased [the eight-site polaron in Fig. 1(b) is stable for $0.148 < J/t < 0.243$] until $\xi \sim J^{-\frac{1}{2}}$, consistent

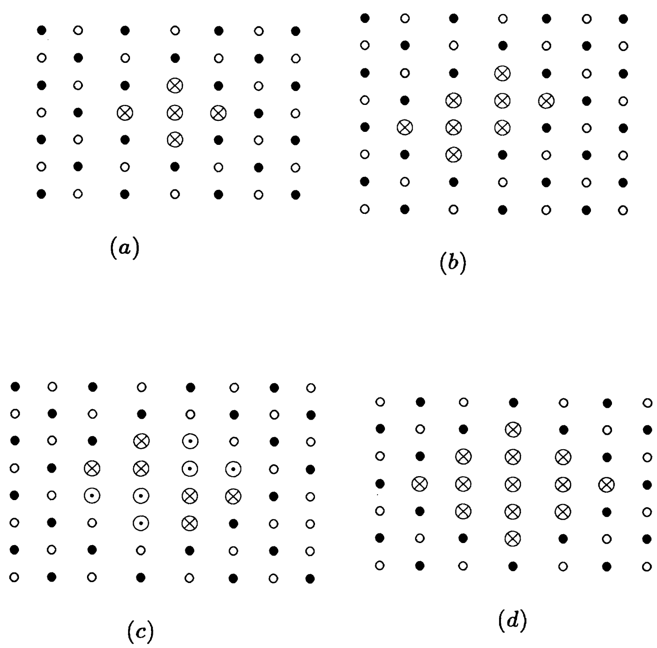

FIG. 1. Polaronic solutions. The symbols ○ and • indicate spin up and spin down, respectively. The symbols ⊗ and ⊙ indicate spin up and spin down, and in addition a nonzero hole density on the site. For the one-hole case we report the small polaron (a), the 8-site polaron (b), and the 13-site polaron (d). For the four-hole case is shown the 2×2 plaquette (c) and the 13-site polaron (d).

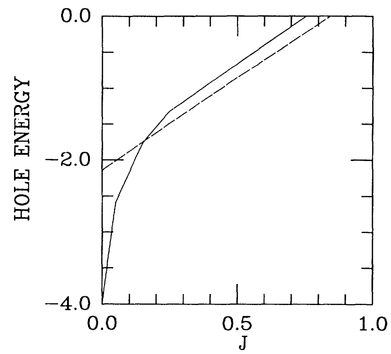

FIG. 2. Variational hole energy in unit of $|t|$ as a function of J on a 10×10 lattice. The dashed line is the semiclassical spiral solution of Shraiman and Siggia with momentum $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$. The solid line represents our large-q mean-field solution: A static polaron of increasing size as J is lowered. The abrupt changes of the energy at small J are due to corresponding first-order transitions to larger and larger polaron size.

with theoretical arguments,[6] so that in the $J/t \to 0$ the polaron solution eventually turns in the Nagaoka state. With the polaron spin background the mean-field energy and the orbital can be easily evaluated analytically. We report the case of the five-site polaron localized at site i_0. Writing the orbital in Eq. (3.17) in the form $\psi(i) = f\delta_{i_0 i} + g_i \Omega_{i_0 i}$, the diagonalization of Eq. (3.15) gives

$$\begin{aligned} \mathcal{E}_0 &= -\frac{J}{2}(2N-4) - 2t\lambda_0, \\ \lambda_0 &= -\frac{3J}{8t} + \mathrm{sgn}(t)\sqrt{1+\left(\frac{3J}{8t}\right)^2}, \\ f &= \frac{1}{\sqrt{1+\lambda_0^2}}, \quad g_i = \frac{\lambda_0}{2\sqrt{1+\lambda_0^2}}. \end{aligned} \tag{4.4}$$

The energy of the antiferromagnet with four missing bonds is recovered in the $J/t \to \infty$ limit, because we have $\lambda_0 \to 0$ so that $f \to 1$, $g_i \to 0$, which means that the hole is statically placed on site i_0. The one-hole energy (referred to the half-filled ground-state energy $\mathcal{E}_{\rm AF} = -JN$) for the Shraiman and Siggia state at momentum $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ and the polaron estimate is plotted in Fig. 2 as a function of J/t in a 10×10 lattice. The comparison of the two energies is meaningful because both represent a variational estimate of the ground-state energy of the t-J model. However, the two variational wave functions refer to different order of approximation, because the hole in the Shraiman and Siggia estimate has a definite momentum. Propagating the polaron through the whole lattice via processes as depicted in Fig. 3 (highly nonperturbative in $1/q$, as discussed in Ref. 21), eventually decreases the energy, but the present data shown in the Fig. 2 clearly indicate that the spiral has lower energy than the static polaron, unless for small J/t.

We consider next the case of four holes. For large J/t the stable state is clearly localized in a 2×2 plaquette [see Fig. 1(c)]. As we decrease J, for $J/t < 1.09$ the four holes prefer to remain localized in a polaron of 13 sites, tilted by 45° with respect to the x, y axes [see Fig. 1(d)], rather than to split into a couple of bound pairs. For J/t smaller and smaller the size of the polaron smoothly increases until the spins are fully polarized in the given finite 10×10 square lattice. These results support the scenario of Emery, Kivelson, and Lin.[6] At least at the mean-field level the classical solution consists of a hole-rich phase fully polarized and a classical antiferromagnetic region which are completely phase separated for arbitrary J. The exact phase boundary in the thermodynamic limit may be obtained by minimizing the energy of the phase separated phase. Following Emery, Kivelson, and Lin we get a critical J_c above which phase separation occurs, given by

$$\frac{J_c(\delta)}{|t|} = \frac{\int_{-4|t|}^{E_F} (E_F - E)N(E)dE}{2B},$$

$$\delta = \int_{-4|t|}^{E_F} N(E)dE, \tag{4.5}$$

$$N(E) = \frac{1}{2\pi^2|t|}K[\sqrt{1-(E/4t)^2}], \tag{4.6}$$

where the spinless fermion density of states $N(E)$ is expressed in terms of the complete elliptic integral of the first kind K, E_F is the spinless fermion Fermi energy at

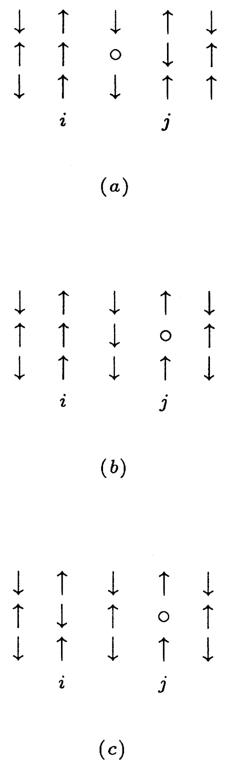

FIG. 3. Second-order process for the $q = \frac{1}{2}$ theory that allows the small-polaron propagation. The wave function $|\Psi_i\rangle$ of the polaron at site i is written as $|\Psi_i\rangle = |f_i\rangle + \sum_k \Omega_{ik}|g_{ik}\rangle$. In (a) we have the state $|g_{ik}\rangle$ entering the polaron at site i. In (b) we have the intermediate state $|\delta_i^j\rangle \sim H_{tJ}|g_{ik}\rangle$ which is a one-particle excited state and corresponds to a local minimum of the energy functional (4.1). In (c) we have the state $|f_j\rangle$ entering the polaron at site j, which is obtained by a further application of the Hamiltonian: $|f_j\rangle \sim H_{tJ}|\delta_i^j\rangle$. Because of $\langle\Psi_i|H_{tJ}^2|\Psi_j\rangle \sim g_i f t J$, for $i \neq j$, an effective intrasublattice hopping is generated.

the corresponding doping δ, and B is the classical energy per bond ($B = 1$) of the Heisenberg antiferromagnet. The resulting phase diagram in the J-ρ plane, where $\rho = 1 - \delta$, is shown in Fig. 4. Here we note the characteristic $\delta \sim \sqrt{J}$ singularity occurring at low doping as the size $\xi \sim J^{-\frac{1}{2}}$ of the polaron increases in a singular way. At low density Eq. (4.5) is valid only if electrons do not form bound states. This is actually the case for the exact t-J Hamiltonian,[6] where two electrons form a bound singlet pair for $J/t > 2$. In this approach, however, the paramagnetic phase at low density is clearly not well characterized since the spins are frozen in some fixed direction. As a result two electrons never bind—as we have tested numerically—and the phase boundary, which is like that of Emery, Kivelson, and Lin, represents the exact mean-field phase diagram. Let us discuss now what happens for $J \leq J_c$ at fixed density. At $J = J_c$ the Nagaoka state is stable by construction since the hole-rich phase exhausts all the allowed space at the given density. It is then easy to convince ourselves that if we decrease J/t the Nagaoka state is even more stable be-

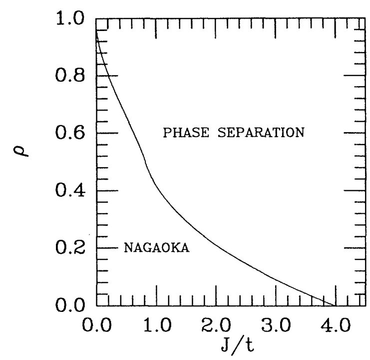

FIG. 4. Phase diagram of the t-J model obtained with the Hartree-Fock large-spin approach.

cause lowering J/t favors the polarized solution.

At the large-spin *mean-field level* we therefore end up with a very simple phase diagram consisting of a ferromagnetic phase for $J \leq J_c$ and a separated phase for $J > J_c$.

V. DISCUSSION AND CONCLUSIONS

In this paper we have presented the coherent states that allow to give a variational foundation to the large-spin limit of the t-J model. These states are obtained by grading according to the spl(2,1) algebra the standard su(2) spin coherent states. We have emphasized how the large-spin limit can be performed in distinct schemes, and applying one of them we have rigorously derived the Kane-Lee-Read Hamiltonian. We have discussed the shortcoming of this approach, related to the fact that in this scheme the mean-field solution turns out to be the classical Néel state, independently from the density. As a consequence phase separation cannot be recovered at the mean-field level.

We then have presented and numerically investigated the effective spinless fermion Hamiltonian obtained by means of a different and more satisfactory definition of the large-spin generalized t-J model. This mean-field model Hamiltonian has the essential properties and symmetries of the original Hamiltonian; in particular, it exactly takes into account the constraint of no-double occupancy. The mathematical tools we have employed are similar to other proposed techniques, notably the Swinger-boson–slave-fermion representation. However, we hope to have better clarified the mathematical and physical assumptions underlying the large-spin limit of the t-J model. More important, by means of the spl(2,1) graded coherent states we have shown that the mean-field solution is independent of the magnitude of the expansion parameter and therefore the corresponding energy is variational. In this way we have generalized a very useful property of the spin systems.

Our numerical investigation confirms that the polaron solutions are the lowest-energy configurations of the t-J model in the large-spin limit. However, we do not find that the static small polaron has lower energy compared to the Shraiman-Siggia spiral state as reported by Auerbach and Larson,[21] at least when in the definition of the t-J model three-site contributions are neglected. The investigation of the full phase diagram at the mean-field level support the picture of Emery, Kivelson, and Lin: In the $J-\delta$ plane a critical $J_c = J_c(\delta)$ with $J_c \to 0$ for $\delta \to 0$ separates the ferromagnetic and the phase-separated phases.

For $J = 0$ the large-spin solution is always fully polarized and our numerical analysis suggests that the instability of the Nagaoka state cannot be found at the mean-field level. The mean-field picture is exact for a single hole, likely for small doping, but is incorrect for large doping, where existing numerical works[22] and the variational singlet Gutzwiller projected wave-function[23] result seems to suggest that the Nagaoka state never survives at finite concentration of holes. On the other hand for $J = 0$ the energy $\mathcal{E}_0$ obtained by minimizing the functional (4.1) has the particle-hole symmetry, i.e., $\mathcal{E}_0(\delta) = \mathcal{E}_0(1-\delta)$. This is not a true symmetry of the infinite-U Hubbard model and thus we expect that $1/q$ fluctuations play a relevant role, especially for small density. Nonperturbative processes may be of some relevance; however, we expect the mean-field picture to be reliable in the large-J/t region.

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