Phase separation and stripes in a boson version of a doped quantum antiferromagnet

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A theoretical investigation of boson versions of the t-J and t-J_z models on the square lattice is carried out, by means of Green's function Monte Carlo simulations. Accurate ground-state energy estimates as a function of hole doping are obtained, allowing one to investigate the stability of the uniform phase against separation of the system into hole-rich and hole-free phases. In the boson t-J_z model, such a separation is found to occur for arbitrarily small values of J_z, at sufficiently low hole doping. Phase separation is suppressed in the boson t-J model, which features a uniform ground state at any doping, for $J/t \lesssim 1.5$. Relevance of this study to the corresponding fermion models is discussed. Fermi statistics *enhances* the tendency toward phase separation; in particular, phase separation at low doping is predicted in the fermion t-J_z model at any $J_z > 0$. The possible formation of stripes of holes is investigated for systems featuring both periodic and cylindrical boundary conditions. No evidence of a striped ground state is found in either the t-J or t-J_z boson models.

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I. INTRODUCTION

The fermion t-J Hamiltonian is defined as

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

The sums run over all pairs of nearest-neighboring (NN) lattice sites; $\hat{c}^{\dagger}_{i,s}$ creates an electron with spin projection s at lattice site i, and $\mathbf{s}_i = \frac{1}{2} \sum_{\alpha\beta} \hat{c}^{\dagger}_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} \hat{c}_{i\beta}$ is the spin operator at lattice site i ($\boldsymbol{\sigma}$ is a vector of Pauli matrices); t is an electron-hopping matrix element; and $\hat{n}_i = \sum_s \hat{c}^{\dagger}_{i,s} \hat{c}_{i,s}$. There is a restriction in the Hamiltonian (1) of no double occupation of any lattice site.

The t-J model describes mobile holes in a quantum antiferromagnet; in two dimensions, it is believed by some to capture the essential physics of the copper-oxide planes of the doped high-T_c compounds.[1] Also intensely studied, in the same context, is the t-J_z model,[2] obtained by replacing $\mathbf{s}_i \cdot \mathbf{s}_j$ by $s^z_i s^z_j$ in Eq. (1). The problem of phase separation (PS) in the ground state of these models is relevant to various theories of high-T_c superconductivity, and is also of considerable fundamental interest.

The suggestion was made for the t-J model that for $J/t > 0$, a state featuring uniform hole density should be unstable against separation into two phases: one rich in holes, the other hole-free.[3] Numerous theoretical calculations have been carried out, purporting to provide a quantitative test of such a prediction; remarkably, however, a decade of intense work has produced no definite agreement. In spite of its deceivingly simple appearance, the t-J model has proven beyond the capability of essentially *all* available quantum many-body methods. A combination of factors, including the fermion character of the model, its strong correlation, and the need to obtain ground-state estimates in the thermodynamic limit, limits the effectiveness of even the most powerful techniques, including high-temperature expansions,[4] Lanczos,[5] and stochastic projection methods,[6–8] as well as the density-matrix renormalization group.[9] This point can be illustrated by noting how not only results obtained with different computational approaches,[4–6,9] but even those produced by similar calculations[6–8] have given rise to conflicting interpretations.[10]

It is sometimes possible to make progress on an intractable problem, by studying a simplified version of it, with the aim of gaining qualitative insight; one might then use physical intuition, analogy, and existing theoretical results, to draw at least some general conclusions for the problem of interest. There are, of course, many possible ways of rendering the t-J model more tractable, by eliminating one or more complicating features; for example, one may resort to a mean-field type description of some of the underlying degrees of freedom. In this work, the simplification arises from a change of quantum statistics of the particles in the model.

Generalized versions of the fermion t-J model, with holes of arbitrary statistics coupled to fermion spin systems, have been investigated by other authors;[11] here, however, *fully bosonic* versions of both the t-J and t-J_z models are considered. That a change of quantum statistics, from Fermi to Bose, should simplify a strongly correlated quantum many-body problem is not obvious; it is so, however, because a powerful computational method exists, known as Green's function Monte Carlo[12] (GFMC), which allows one to compute ground-state thermodynamic properties of interacting Bose systems, with essentially no approximations. This method has been utilized, over the past three decades, to investigate a wide variety of quantum many-body problems.[13] While it provides virtually exact results for Bose systems, its application to fermions is hampered by the well-known sign problem, for which, presently, some workarounds are available,[14] but, it seems fair to state, no definite solution.

A study is presented here of PS in the ground state of boson versions of the t-J and t-J_z models. The formation of stripes of holes, a scenario proposed by some authors for the fermion t-J model,[9] is also explored in these Bose Hamiltonians. Accurate numerical results are obtained using the GFMC method, on square lattices of relatively large size (up to 1024 sites). The boson models incorporate much of the same physics of their fermion counterparts; the theoretical issue is to extract information on the fermion models, based on results obtained for the boson systems.

The main conclusions of this work are the following:[15]

(a) Fermion Hamiltonians are closer to a PS instability than their boson counterparts.

(b) In the boson version of the t-J_z model, separation into hole-rich and hole-free phases occurs, at sufficiently low hole doping, for arbitrarily small values of J_z/t. It is proposed, based on point (a), that this conclusion *a fortiori* should hold for the fermion t-J_z model.

(c) Phase separation is suppressed in the boson t-J model, which features a uniform ground state for $J/t \lesssim 1.5$. Contrary to what is commonly assumed, the physics of the t-J and t-J_z models differ significantly in the low-doping limit.

(d) No evidence of a striped ground state is ever found in either boson model.

Although the conclusions about PS or stripe formation cannot be directly extended to the fermion t-J model (at least not in any obvious way), they show that, if PS or stripes do indeed occur, Fermi statistics must play a crucial role, i.e., these effects are not merely the result of a simple energy interplay.

This paper is organized as follows: in the next section, the models of interest are introduced and motivated; in Sec. III, the computational methodology utilized is briefly reviewed; in Secs. IV and V results are presented for PS in the boson t-J_z and t-J models. In Sec. VI, the basic energetics of fermion and boson models are compared, and arguments are offered to the effect that fermion models are closer to a phase separation instability; this allows one to draw a definite conclusion on PS in the fermion t-J_z model. The search for stripes in both boson models is described in Sec. VII, and conclusions are presented in the last section.

II. THE MODEL

The goal is to define a boson equivalent of the fermion t-J (and t-J_z) model. Because the t-J Hamiltonian can be obtained via a strong-coupling expansion of the fermion Hubbard model,[16] a reasonable starting point seems the following, Hubbard-like Hamiltonian of a mixture of two different species of bosons, of equal masses, interacting via an on-site repulsive potential:

$$\hat{H}_o = -t\sum_{\langle ij\rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j + \text{H.c.}) + V\sum_i (\hat{n}_i^2 + \hat{m}_i^2) + U\sum_i \hat{n}_i \hat{m}_i , \qquad (2)$$

where $\hat{H}_o$ is defined on a square lattice of $N = L\times L$ sites, with periodic boundary conditions. The hopping integral t, as well as the on-site potential energies V and U, are all positive; $\hat{a}_i^\dagger$ and $\hat{b}_i^\dagger$, are boson creation operators for species A and B at site i, and $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ and $\hat{m}_i = \hat{b}_i^\dagger \hat{b}_i$ are corresponding number operators. Let N_A and N_B be the number of particles for the two species. For definiteness, it is assumed all throughout that $N_A = N_B \leqslant N/2$. The particle density is defined as $\chi = (N_A + N_B)/N$, where the hole density $h = 1 - \chi$. The two Bose species play the role of electrons of spin up and down in the fermion Hubbard model; in that case, Pauli principle limits site occupation to up to one particle of a given spin. The same effect can be obtained in Eq. (2) by setting $V = \infty$, i.e., by assuming a hard-core, on-site repulsion between bosons of the same species. Thus, a lattice site can only be doubly occupied by two different bosons. Note that, while there is no clear relationship to high-T_c superconductivity, $\hat{H}_o$ is neither unphysical nor implausible. With $V = \infty$, and in the strong-coupling limit ($U \gg t$), it reduces to the following effective Hamiltonian:

$$\hat{H} = -t\sum_{\langle ij\rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j + \text{H.c.}) - \frac{1}{2}\sum_{\langle ij\rangle} (J_z[\hat{n}_i \hat{m}_j + \hat{m}_i \hat{n}_j] + J_\perp \hat{P}_{ij}), \qquad (3)$$

where $J_z = J_\perp = 4t^2/U$ and where $\hat{P}_{ij}$ is an operator exchanging a particle of type A (B) at site i with a particle of type B (A) at site j. The Hamiltonian (3) is defined in the subspace in which no double occupation of sites is possible. This procedure, applied to the fermion Hubbard model, leads to the standard fermion t-J model, Eq. (1), upon neglecting a three-site term, also neglected here. The energy scale is taken to be t, henceforth set equal to one. Of interest here is the ground state of a generalized version of Eq. (3), in which J_z and $J_\perp$ are treated as independent parameters. Specifically, two different cases are considered: (a) $J_z = J$ and $J_\perp = 0$, referred to as the boson t-J_z model, and (b) $J_z = J_\perp = J$, referred to as boson t-J model.

As mentioned above, the fermion versions of these models describe the motion of holes in an antiferromagnetic spin background; in the t-J_z model, the spin background is rigid, whereas quantum fluctuations are present in the t-J model. The t-J_z model is often studied as a simplified version of the t-J, on the assumption that it should retain most of its essential physics.[2,17] This is particularly expected to be the case in the $J \to 0$ limit, in which quantum spin fluctuations may not play too important a role.

III. COMPUTATIONAL METHODOLOGY

The study of the Hamiltonian (3), for different values of the parameter J and as a function of the hole density h, has been carried out in this work using standard GFMC. Because this is a rather well-established technique, extensively discussed in a number of articles,[13] implementational details will not be reviewed here.

The projection operator used is $\hat{G} = E - \hat{H}$, where E is a constant which must be $\geqslant E_M$, the largest eigenvalue of $\hat{H}$; an upper bound for E_M is easily determined. A population of typically 300 walkers was utilized, which was found to give undetectable bias in the estimates, within the statistical uncertainties of our calculation.

Just as for any Bose system, no sign problem arises with the Hamiltonian (3), as all off-diagonal elements of the projection operator $\hat{G}$ are positive. This allows for a stable algorithm and projection times long enough that reliable ground state estimates can be obtained. A Jastrow many-body wave function was utilized, both as trial and guidance function:[13]

$$\Psi(c)=\exp\left[-u\sum_{\langle ij\rangle}(n_in_j+m_im_j)\right], \tag{4}$$

where $|c\rangle\equiv|n_1n_2\cdots n_Nm_1m_2\cdots m_N\rangle$ is a generic configuration of the system, specified by the number (0 or 1) of bosons of either species at every lattice site, and u is a variational parameter, whose optimal value was adjusted by minimizing the variational energy estimate provided by the trial state, Eq. (4). Unbiased estimators[18] were used for all observables. This is an important aspect, as estimates for observables other than the energy can often have a significant bias, if the usual "mixed estimators" are adopted.

In order to investigate the occurrence of PS in the ground state of Eq. (3), accurate estimates are needed of the ground-state energy per site $E(h)$ of the uniform phase, as a function of the hole concentration h. Specifically, the system is unstable against PS below a critical hole concentration h_c if

$$E(h)\geqslant\frac{(h_c-h)E(0)+hE(h_c)}{h_c} \tag{5}$$

for $0\leqslant h\leqslant h_c$. If condition (5) holds for any hole concentration below h_c the system will separate into two phases, one with hole concentration h_c, the other with no holes. Condition (5) is clearly equivalent to the presence of a minimum, at h_c, of the energy per hole $e(h)$, defined as

$$e(h)=\frac{E(h)-E(0)}{h}. \tag{6}$$

GFMC simulations are suitable to investigate PS based on Eq. (5), for they allow the computation of $E(h)$ on finite lattices, where the ground state of Eq. (3) necessarily features a uniform hole density.

IV. RESULTS FOR THE t-J_z MODEL

Let us consider first the results obtained with $J_\perp=0$, namely for the t-J_z model. This is the simplest Hamiltonian of a mixture of hard-core bosons, with a NN attraction between unlike species.

Figure 1 shows results for the ground-state energy per hole $e(h)$ (in units of t) in the boson t-J_z model, as a function of the hole density, on an 8×8 lattice, at different values of $J_z=J$. With the sole exception of the $J=0$ case, the $e(h)$ curves feature a well-defined minimum at a finite hole concentration, signaling the instability of the homogeneous phase, which is stable at all h only at exactly $J=0$.

Calculations on lattices of different sizes were carried out, 32×32 being the largest. Figure 2 shows estimates for $e(h)$ on various lattices, at $J=0.1$ and $J=0.05$. Although finite-size effects are apparent, the presence and the position of the minimum for $e(h)$ at low hole density can be established rather comfortably on an 8×8 lattice. Extrapolation of the results to the thermodynamic limit ($L\to\infty$) yields estimates indistinguishable, within statistical errors, from those obtained on a 32×32 lattice.

The lowest value of J considered here is $J=0.05$; as $J\to 0$, calculations on larger lattices are needed, in order to establish whether PS occurs. This is because the critical concentration also approaches zero, and reliable numerical energy estimates require a sufficient number of holes in the system.

Figure 3 shows the phase diagram of the boson t-J_z model, constructed using the data obtained in this work. The dashed line is a fit to the values of the critical concentration h_c, based on the expression $h_c(J)=\alpha\sqrt{J}$, which can be jus-

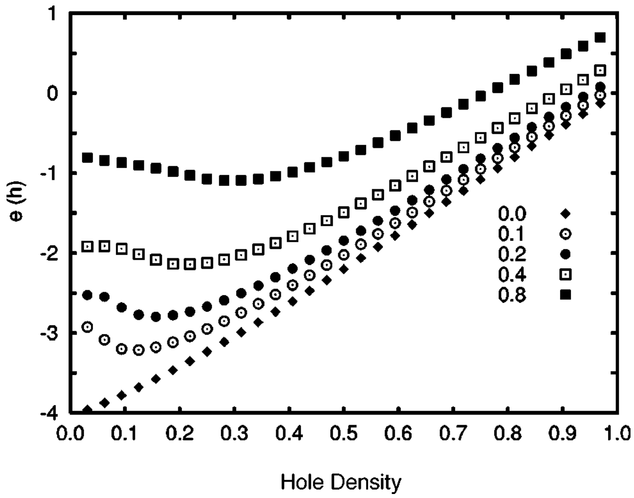

FIG. 1. Ground-state energy per hole $e(h)$, as a function of the hole density h, for the Hamiltonian (3), with $J_\perp=0$ and $J_z=J$ (boson t-J_z model), at different values of J on an 8×8 lattice. Statistical errors are smaller than symbol sizes. There is a minimum at finite hole density, for all nonzero values of J, which signals the separation of the system into hole-rich and hole-free phases.

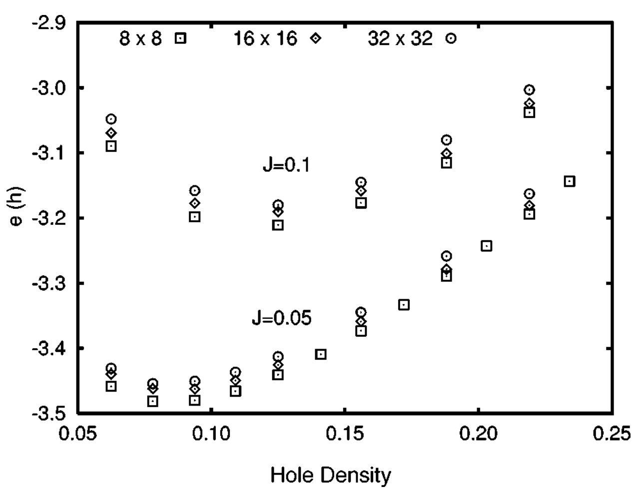

FIG. 2. Ground-state energy per hole $e(h)$, as a function of the hole density h, for the Hamiltonian (3), with $J_\perp=0$ and $J_z=J$ (boson t-J_z model), at $J=0.1$ (upper data points) and $J=0.05$ (lower data points), and on square lattices of different sizes. Statistical errors are smaller than symbol sizes.

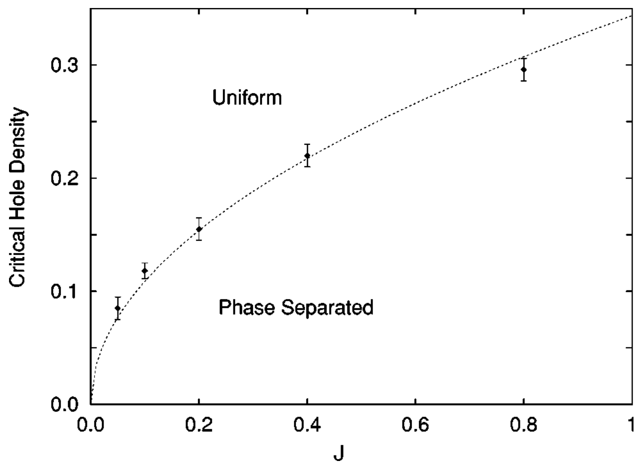

FIG. 3. Proposed phase diagram of the boson t-J_z model. Diamonds show critical hole densities as a function of J. Below the dashed curve, the system separates into hole-rich and hole-free phases. The dashed curve is a fit to the diamonds, obtained using the expression $h_c(J) = \alpha\sqrt{J}$.

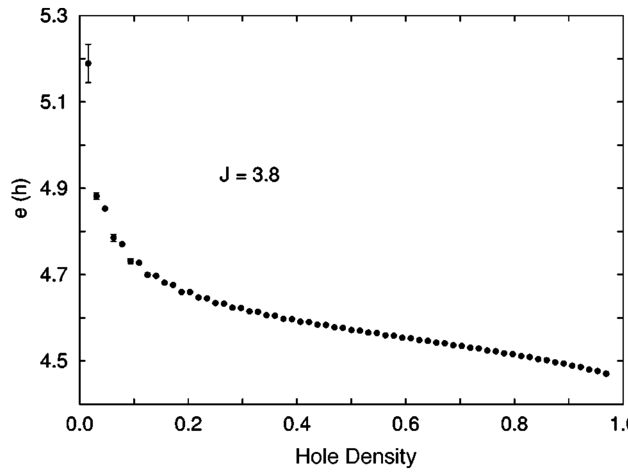

FIG. 4. Ground-state energy per hole $e(h)$ as a function of the hole density h, for the boson t-J Hamiltonian, with $J = 3.8$ on an 8×8 lattice.

tified theoretically in the low doping limit.[3] The excellent fit to the data provides support to the PS scenario.

Of course, all of this evidence is, to some extent, circumstantial. A numerical calculation such as the one performed here cannot prove, in a strict mathematical sense, that PS occurs at arbitrarily low values of J. At the same time, the results furnished here arguably provide as robust an evidence of such a conclusion as can be obtained numerically, for strongly correlated many-body Hamiltonians such as the ones considered here.

More important, is that the occurrence of PS at arbitrarily low values of J can be physically explained based on the following, simple physical argument: For an arbitrarily small, but finite, value of J, the system finds it energetically favorable, at sufficiently low-hole doping, to separate into two phases: one features "antiferromagnetic" order, each site with a boson of type *A (B)* being surrounded by NN sites occupied by bosons of type *B (A)* and no holes; the other phase is rich in holes, which frustrate the staggered order with their motion. These considerations are completely independent of quantum statistics, and it is therefore reasonable to expect a similar scenario in the fermion t-J_z model (more on this point in Sec. VI).

V. RESULTS FOR THE t-J MODEL

Let us now examine the physics of the boson t-J model, that is, the system described by Eq. (3) with $J_\perp = J_z = J$. The presence of the exchange term ($J_\perp$) does not complicate significantly the GFMC calculation; the same wave function, Eq. (4), is used.

PS in this model can be easily observed at relatively large values of J, much like in the fermion model. In this limit, the system attempts to lower its energy by minimizing the number of broken antiferromagnetic bonds, and quantum statistics is essentially irrelevant.

Figure 4 shows results for $e(h)$ at $J = 3.8$; the minimum of the curve is at $h = 1$ (no holes), i.e., there is complete separation between holes and particles at any hole density. Analytical calculations[19] for the fermion t-J model yield a value of $J = 3.4367$ above which such complete PS occurs. Such an estimate is based on a comparison of the ground-state energy of the fully phase separated state, with that of a gas of bound pairs of electrons (s-wave singlets). The same argument carries over to the boson t-J model, with s-wave pairs formed by two bosons of different species. Numerical results obtained in this work are consistent with the above value of J as the threshold for complete PS in the boson t-J model as well.

As J is decreased, however, there is strong a suppression of PS in the boson t-J model, both with respect to the boson t-J_z as well as the fermion t-J models. For example, Fig. 5 shows results at $J = 2.5$; the curve has a minimum at around $h \approx 0.08$, though its precise location is difficult to pinpoint, as the minimum becomes less and less well defined, as the lat-

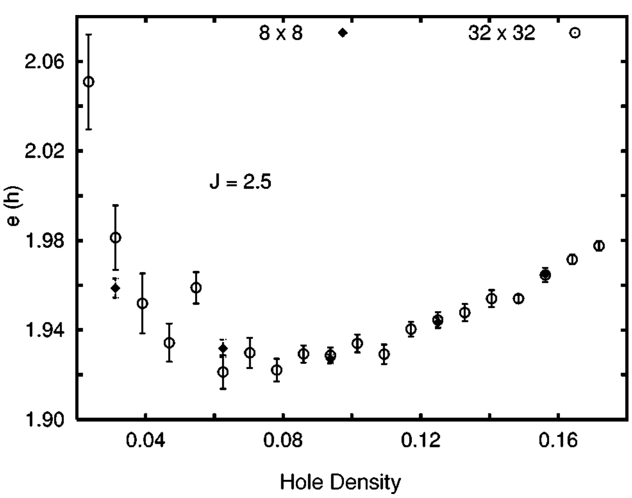

FIG. 5. Ground-state energy per hole $e(h)$ as a function of the hole density h, for the boson t-J Hamiltonian, with $J = 2.5$ on an 8×8 (filled diamonds) and on a 32×32 (open circles) lattice.

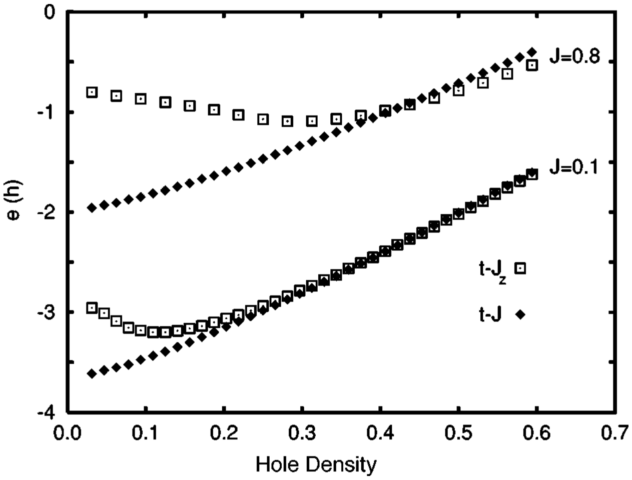

FIG. 6. Ground-state energy per hole $e(h)$ as a function of the hole density h, for the boson t-J_z (boxes) and boson t-J model (diamonds), with $J=0.8$ (upper curves) and $J=0.1$ (lower curves), on an 8×8 lattice. Statistical errors are smaller than symbol sizes.

tice size is increased.[21] In order to find a similar value of h_c for the boson t-J_z model, one needs to consider values of J as low as 0.05 (see Fig. 2), confirming the strong suppression of PS in the boson t-J model, with respect to the boson t-J_z. In the fermion model, the critical hole density at $J=2.5$ is estimated[6] at $\approx 70\%$, i.e., the suppression of PS in the boson t-J model is clear and significant even in comparison to the fermion equivalent. In Fig. 6 the quantity $e(h)$ is shown for both the boson t-J and t-J_z models, at $J=0.8$ and $J=0.1$. Whereas, in the t-J_z model, PS occurs at low h, the monotonic behavior of $e(h)$ for the t-J model indicates that the uniform phase is stable at all hole concentrations.

Note how, for $J=0.1$, at $h\gtrsim 0.2$ the estimate for $e(h)$ is essentially identical in both models. This is in agreement with the generally held belief that, at low values of J, quantum fluctuations associated to the exchange part of Eq. (3) should not play an important role. However, at sufficiently low hole density the presence of the exchange term renders the physics of the two models *qualitatively different*.

One may understand the different behavior of the t-J_z and t-J models, in the low doping limit, based on the "string" picture.[2] In the t-J_z model, a hole leaves behind, in its motion, a string of bosons of either species, displaced by one lattice site. Thus, in the t-J_z model the separation of the system into hole-rich and hole-free phases becomes energetically advantageous, at low hole density, as a way to limit the damage caused by the holes to the antiferromagnetic order. In the t-J model, however, quantum fluctuations associated with the $J_\perp$ term of Eq. (3) mend the damage due the hole motion, restoring local order.[20] Again, these considerations are completely independent of quantum statistics, i.e., apply to the fermion models as well.

An analysis of the results obtained on an 8×8 lattice suggests that the ground state of the boson t-J model should feature a uniform phase (no PS) at all h for $J\lesssim 1.5$. In other words, a finite value $J_{\rm cr}$ of J exists, approximately equal to 1.5, below which the ground state is uniform at all dopings. In principle, of course, this result should be confirmed by a set of calculations carried out for much larger lattices. This was not pursued in this work, however, because the case for a strong suppression of PS in the boson t-J model, with respect to both the boson t-J_z and the fermion t-J models seems solid, regardless of whether $J_{\rm cr}$ is finite or not; this is, in our view, the relevant physical conclusion.[22] It should also be noted that the accurate computation of $e(h)$ at low h becomes problematic on large lattices, even in the absence of the sign problem. This is because the subtraction of two large numbers is required, each one with a relatively large associated uncertainty.

VI. COMPARISON OF FERMI AND BOSE HAMILTONIANS AND IMPLICATIONS FOR PHASE SEPARATION

What do these results suggest, regarding PS in the fermion t-J_z and t-J models ? Obviously, great care must be exercised in assessing the relevance of any boson model to its fermion counterpart.

Let us begin with the t-J model. Broadly speaking, PS between hole-rich and hole-free phases is clearly observed, at hole densities $\gtrsim 0.05$, only at relatively large values of J ($\gtrsim 2.0$). This is in contrast with the fermion t-J model, for which practically all theoretical studies predict PS, at these low hole densities, at considerably lower values of J (for J less than 1 in most numerical studies).

Furthermore, numerical results obtained here suggest that the uniform phase is thermodynamically stable, in the boson model, for $J<1.5$. On the other hand, for the fermion t-J model most theoretical investigations[7,8] yield estimates of $J_{\rm cr}<1$, the highest[4] being ~ 1.2, the lowest being zero.[6] All of this suggests that in the fermion model the tendency to hole PS is enhanced, with respect to the boson model.

This point can be illustrated by comparing estimates for the ground-state energy per site, $E_B(h)$ and $E_F(h)$, as a function of hole concentration, for the Bose and Fermi cases. PS is signalled by a negative curvature of this function.[23] For both the t-J and the t-J_z case, it is $E_B(h)\leqslant E_F(h)$, i.e., the Bose energies are strict lower bounds for the Fermi energies. Also, $E_B(0)=E_F(0)$ and $E_B(1)=E_F(1)$, i.e., at zero and full doping the distinction between Fermi and Bose statistics disappears, in these models. An upper bound for both $E_B(h)$ and $E_F(h)$ is provided by the energy of the fully separated state $[E_{\rm PS}(h)]$, in which the two phases contain, respectively, no holes and no particles. Because $E_{PS}(h)$ has zero curvature, in general the curvature of $E_B(h)$, at low h, will be greater than that of $E_F(h)$, i.e., the fermion model will be closer than the boson to a PS instability. This is noteworthy, as it seems counterintuitive. Fermi statistics, which causes an effective repulsion among particles, is normally assumed to favor mixing, i.e., demote PS.

As an example, Fig. 7 shows both $E_B(h)$ and $E_F(h)$, for the t-J model, at $J=1$, as well as the energy of the fully separated state (dotted line). Estimates for the fermion case are taken from several numerical studies, all based on GFMC.[6,8,24] The curvature at low h is clearly very different for the two cases, much greater for bosons than for fermions. It seems reasonable to expect that this should be the case at any value of J. In both cases (boson and fermion) there is a

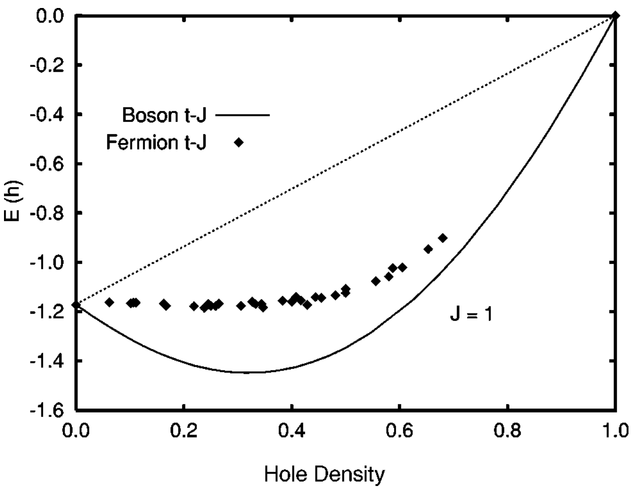

FIG. 7. Ground-state energy per site $E(h)$, as a function of the hole density h, for the boson (solid line) and fermion (diamonds) t-J Hamiltonian, with $J=1$. Results for the fermion case are from Refs. 6 and 24. The dotted line corresponds to a fully phase separated system. Statistical errors are smaller than the diamonds, and are of the order of 0.001 for the solid line.

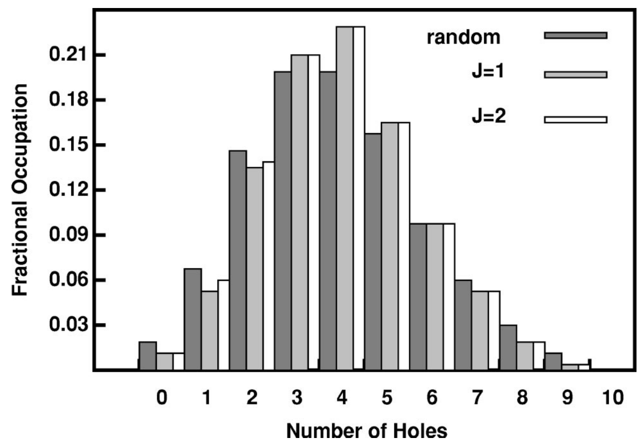

FIG. 8. Fractional occupation by holes of rows (columns) of a 32×32 lattice, in the ground state of the boson t-J model. The hole density is 0.125 (128 holes), and $J=1$ (white columns) and 2 (gray columns). Statistical errors are typically of the order of 1%. Dark columns correspond to random placement of holes in the lattice.

competition between the minimization of the number of broken "antiferromagnetic" bonds, which promotes hole clustering, and thus PS at large J, and the delocalization of the holes, which favors the uniform phase. However, the exchange energy increases, in the fermion case, the energy cost of injecting holes in the antiferromagnetic background, thereby rendering the uniform phase less competitive than in the boson system, for a given value of J.

The above considerations do not allow one to draw a definitive quantitative conclusion regarding PS in the fermion t-J model. Let us, however, consider the fermion t-J_z model. No quantitative study of its energetics, at finite hole concentration, has been carried out so far. Because PS, at sufficiently low h, is observed for arbitrarily small values of J, in the boson Hamiltonian, it will *a fortiori* occur in the fermion t-J_z model, at the same physical conditions. Moreover, the values of the critical hole concentrations below which PS occurs in the boson model should provide lower bounds for the corresponding concentrations in the fermion case. For example, looking at Fig. 1 one may expect that, at $J=0.4$, the uniform phase will be stable at hole concentrations $\gtrsim 0.25$; at $J=0.2$, the critical hole concentration is $\gtrsim 0.15$. These values of J and hole concentrations are well within the so-called physical range, in which the t-J_z model is believed to capture some of the essential physics of the cuprate superconductors. Based on the results presented here, only at very small values of J ($\lesssim 0.05$) is the uniform phase expected to be stable, in the fermion t-J_z model, at values of hole doping (~ 0.1) for which superconductivity is experimentally observed.

VII. STRIPES

The formation of "stripes" of holes along a lattice row (or column) has been observed in numerical simulations of the t-J model based on density-matrix renormalization group (DMRG).[9] Some analytical studies of the fermion t-J_z model have also supported the stripe hypothesis.[25] Other numerical studies, however, based upon different methods, have failed to provide the same evidence,[26] and this prediction remains controversial.

There is no agreement as to what energy mechanism should promote the formation of stripes of holes, nor what the specific role of quantum statistics should be. It appears appropriate, therefore, to investigate stripe formation in the boson models as well.

An extensive search for stripes was carried out, in this work, for both the bosonic t-J and t-J_z models, at hole concentrations $h=0.125$ and $h=0.250$. A simple way of detecting the occurrence of stripes, is to histogram the hole occupation of rows (columns) in the ground state, and compare it with what one would expect based on random hole placement. Generally speaking, stripe formation should be signaled by a significantly greater than random probability that (a) empty rows are present, and (b) numbers of holes greater than average occupy the same row. This procedure renders it possible, in principle, to observe stripe formation even if periodic boundary are utilized.

Figure 8 shows histograms of occupation, by number of holes, of the rows (columns) of a 32×32 lattice, with periodic boundary conditions, in the boson t-J model, at a hole density of 0.125. Results are shown for two values of J, namely $J=1,2$; for comparison, the fractional occupation that one would observe if holes were randomly placed throughout the lattice is also shown. The first thing to be noticed is the similarity of the results for the two different values of J. In fact, results for several other values of J, in the interval $0.5\leqslant J\leqslant 2.5$ were obtained, essentially identical to those shown in the figure. Also, results for the t-J_z model are found to be practically indistinguishable than those for the t-J.

The probability $P(l)$, for a cluster of l holes to occupy the same row (column), is found to be significantly greater than random for $l=3,4,5$, and lower than random for all other values of l. This does not seem to support the stripe scenario, given that the average numbers of holes per row (column), in the case considered, is 4; also noteworthy is the fact that the probability of observing empty rows (columns) is actually lower than random. The results of Fig. 8 suggest a rather uniform hole distribution, with small fluctuations around the average of the number of holes per row, or column. The results obtained at $h=0.250$ are qualitatively similar, i.e., they provide no evidence of stripe formation.

In order to compare results more directly with those obtained in Ref. 9, simulations on rectangular lattices (e.g., 4×24) with cylindrical boundary conditions were also carried out. Because translational invariance is broken, one can, in this case, observe directly the formation of stripes by looking at the hole density along the direction in which open boundary conditions are applied.[9] It is interesting to note that these simulations too failed to provide any evidence of stripe formation. On the one hand, this supports the conclusion that the ground state of the bosonic models is not striped. At the same time, it suggests that the mere use of open boundary conditions along one direction is insufficient to stabilize stripes.

VIII. CONCLUSIONS

Boson versions of the t-J and t-J_z models have been studied in this work. Although the main motivation was to extract some information about PS and stripes in the corresponding fermion models, it should be remarked that the phase diagram of isotopic Bose mixtures is certainly of fundamental interest and relevance to various areas of physics.

The Bose Hamiltonians studied here are not directly related to any known high-T_c compound (to the author's knowledge), but can be studied by means of Green's function Monte Carlo without sign problem. This allows one to obtain robust numerical results, difficult to obtain for the fermion models, which have been studied extensively, during the past decade, as simple archetypal models of high-T_c superconductivity.

By studying the physics of the boson systems, interesting physical conclusions may be inferred, some relevant to the fermion models as well. Perhaps the most important conclusion is that a commonly held assumption, namely that the t-J and t-J_z models should feature qualitatively similar behavior, is in fact not valid at low hole density, where the two models display rather different behavior. In particular, PS is much more prominent in the t-J_z than in the t-J model.

Another interesting conclusion is that the fermion models are closer to a PS instability than their boson counterparts. This allows one to predict that PS between hole-rich and hole-free phases will occur, in the fermion t-J_z model, at arbitrarily small values of J_z, for sufficiently low hole concentration. The critical hole concentrations found in the boson t-J_z Hamiltonian, which are lower bounds for the corresponding hole concentrations in the fermion t-J_z, suggest that PS is very robust in this model, including at values of J and hole concentrations considered appropriate to high-T_c superconductivity. This may therefore raise some questions about the fermion t-J_z model as a realistic model of the high-T_c compounds. On the other hand, this study provides no definitive conclusion for the fermion t-J model, regarding PS in the physically relevant region.

An aspect of the boson models that was not considered here, but may have some relevance in the understanding of the phase diagram of the fermion models as well, is the formation of pairs of holes. There is in principle no reason why two holes may not form a bound state in the boson t-J model, in some range of values of J; an interesting issue arises of whether an intermediate phase of hole pairs may exist, between the uniform and phase separated phases. This problem, relevant to some proposed theoretical scenarios of high-T_c superconductivity,[10] will be addressed in future work. A study of hole binding must be carried out in the $h\to0$ limit, and is therefore more challenging than one at finite hole density.

An extensive search for stripe formation in the boson models has been carried out, at hole concentrations of 0.125 and 0.250. None of the simulations performed in this work have provided any evidence of stripes, in a wide range of model parameters. Thus, if stripes do indeed form in the fermion models, they are, much like PS, a direct consequence of Fermi statistics, and not of a simpler energy interplay. In particular, stripes have been alleged to form, in the fermion models, as a result of the attraction of bound pairs of holes.[27]

A final remark: since the bosonic t-J model can be studied by GFMC with no sign problem, it may be worthwhile to obtain results for it also using the other methods that have been used to investigate the fermion model, such as high-temperature expansion, or DMRG. This may provide an unbiased comparison of the reliability of the various techniques.

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