Ground-state energy and spin of a generalized-statistics t-J model

M.W. Long
School of Physics, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom

X. Zotos
Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Postfach 6980, D-7500 Karlsruhe 1, Federal Republic of Germany and Institut Romand de Recherche Numérique en Physique des Materiaux (IRRMA) PHB-Ecublens, CH-1015 Lausanne, Switzerland *

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By analytical and numerical diagonalization methods we examine the dependence of the ground-state energy and spin of a system of holes of arbitrary statistics coupled to a spin system with dynamics as given by a t-J Hamiltonian. We establish exact energy inequalities for the ground-state energy and spin for $J/t = 0$ and $J/t \to \infty$ as a function of hole statistics and present numerical results for intermediate values of J/t. We also discuss Nagaoka's theorem in this generalized context and the mechanism for the apparent inversion of the hole statistics: At $J/t = 0$ bosons have the lowest energy in the ferromagnetic (Nagaoka) ground state, while as $J/t \to \infty$ fermions have the lowest energy in a low-spin-correlations ground state.

I. INTRODUCTION

The motion of holes in a dilute antiferromagnet has recently attracted a great deal of attention. The canonical model to study is the two-dimensional t-J model.[1] One issue discussed is the influence of the spin environment on the motion of the charge carriers (the holes), in particular the statistics of the charge and spin quasiparticles.[2,3] One way to consider the t-J model is as a gas of holes with their own independent statistics coupled to a spin background through the kinetic energy term. In general we can consistently define the statistics of the holes in a two-dimensional system to vary from bosonic to fermionic by imagining the holes pierced with fluxes.[4] Without the spin environment, for instance, a gas of bosons has a lower energy than a gas of fermions. We can then examine how the presence of spins influences this energy relation (or the hole-hole correlations), as a function of spin coupling J/t and hole density. Of course for arbitrary statistics this amounts to generalizing the t-J model.

To study these questions we will consider the hole and spin dynamics as given by the t-J Hamiltonian but we will vary the statistics between the holes in order to probe the actual state of the hole wave function. For fermionic or bosonic statistics there is particle-hole symmetry, which ensures that either particles or holes can carry the statistics. In similarity to the perovskite superconductors, where a small concentration of holes carry the current, we have elected to give the holes the statistical phase for general statistics, thereby using a rather different model from that which has previously been used.

This work is divided in two parts; in the first part, to exemplify our main points, we present the results of a numerical exact diagonalization study on a 4 by 4 lattice followed by results on the ground-state spin for 2 by N lattices, $J/t = 0$ and varying hole concentration. Next we discuss them in terms of an elementary exchange of holes in the presence of spins on a plaquette. In the second part we extensively discuss how to consider the hole-spin wave function and we give analytical arguments to explain the behavior of the ground-state energy and spin for arbitrary hole density for $J/t = 0$ and $t/J \to 0$. In the Conclusions we discuss the limitations of our study and its implications regarding other studies on this problem.

II. NUMERICAL CALCULATIONS

We will consider only two-dimensional bipartite lattices. It is known that the t-J model can be represented in two equivalent ways; in the first the spin degrees of freedom are carried by fermions and the holes satisfy boson statistics with the constraint of no double occupancy (the slave-boson representation) or in the second the spin degrees of freedom are carried by bosons and the holes satisfy fermion statistics (the slave-fermion representation). As we are interested in a numerical calculation, the most appropriate representation is the second one where we do not have to keep track of the phase associated with the spin states, so we attach the statistics to the holes. Then in the generalized t-J model that we study, we treat the holes as hard-core bosons carrying a flux so that when two holes exchange the hole wave function is multiplied by $e^{i\phi}$. The usual t-J model then corresponds to the value $\phi = \pi$, that of fermionic holes. As we mentioned above, we can transfer the statistics from holes to spin degrees of freedom and obtain equivalent models only at the values $\phi = 0, \pi$.

To settle the coupling constants the Hamiltonian we consider, at the original fermionic point, is

$$H = -t \sum_{<ij>s} (\tilde{c}^\dagger_{is}\tilde{c}_{js} + \text{H.c.}) + J \sum_{<ij>} (\mathbf{S}_i \cdot \mathbf{S}_j - n_i n_j/4), \quad (1)$$

where $\tilde{c}_{is}(\tilde{c}^\dagger_{is})$ are annihilation (creation) operators of a fermion on site i with spin s and the tilde implies the restriction to single occupancy. The sum is over all bonds $< ij >$ of a two-dimensional lattice. As we explained above we actually use a representation of bosonic spin degrees of freedom and fractional statistics ϕ for the holes (so the Hamiltonian as written above corresponds to $\phi = \pi$). The first lattice we studied has 4 by 4 sites with open boundary conditions, because of known problems in accommodating fractional statistics in a torus geometry,[5] with two holes. The calculation is performed using a Lanczos method.

In Fig. 1 we present the results for the ground-state energy as a function of the statistical flux ϕ. Again $\phi = \pi$ corresponds to the usual fermionic t-J model. There are three distinct regions in the behavior as a function of J/t. First for $J/t = 0$ the spin of the ground state is maximum (a Nagaoka state) for $\phi < 0.7$ and then the spin cascades to zero for $\phi = \pi$, as is known for the t-J model with two holes.[6] In this regime therefore (for $\phi < 0.7$) the two holes behave according to their nominal statistics as far as their energy dependence on statistics is concerned. With a dashed line we also show the energy of the holes in a completely spin-polarized system (Nagaoka state) to demonstrate that fermionic holes enforce lower spin in order to minimize their energy.

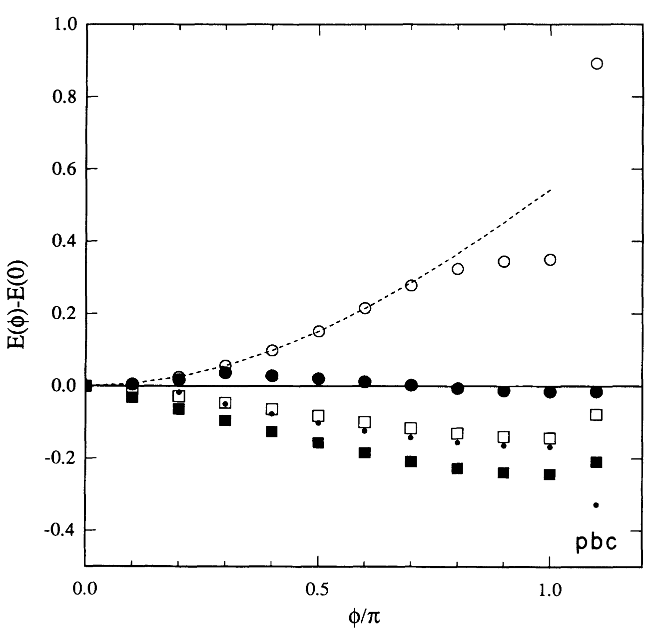

FIG. 1. Difference of ground-state energy $E(\phi)-E(\phi=0)$ as a function of ϕ for different values of J/t for 4 by 4 lattice with 2 holes; $J/t = 0$ (empty circles), $J/t = 0.2$ (solid circles), $J/t = 0.4$ (empty squares), $J/t = 1.0$ (solid squares), $J/t = 4.0$ (dots). Above "pbc" the equivalent points for the lattice with periodic boundary conditions. With dashed line the energy of holes in a completely spin-polarized state (Nagaoka state).

There is a second region for small $J/t \simeq 0.2$ where the spin of the ground state is zero but the energy is not a monotonic function of ϕ. It is rather difficult to say something about this region as it is probably very dependent on finite-size effects. Finally for larger values of J/t the spin of the ground state is zero, the energy is a monotonic function of J/t with the point $\phi = \pi$ the minimum. This result seems as an inversion of the hole statistics. In opposition to a system without spin background, the energy of the hole-spin coupled system has higher energy for bosonic holes than fermionic ones. Therefore the holes in the original t-J model behave rather like hard-core bosons. At first sight it may seem contradictory that we are suggesting that fermions behave more like bosons than bosons do. It is the spin environment which causes the difficulties. We have three systems in mind for comparison: fermions moving in a bath of spins, bosons moving in a bath of spins, and finally spinless bosons moving in isolation. The conclusion that we will wish to suggest is that as $J/t \rightarrow \infty$, fermions moving in a low-spin background behave more like spinless bosons than bosons moving in a low-spin background.

Three main observations are borne out of this calculation; first for $J/t = 0$ the system with bosonic holes has lower energy than the fermionic one, second for $J/t = 0$ the maximal spin occurs for bosonic holes; third for finite J/t the spin is zero and the bosonic point lies higher in energy than the fermionic one. Certainly the system we studied is extremely small and could be argued that the results are characteristic of this cluster. We verified that these three main observations hold for other bipartite lattices with a different number of holes provided that the spin in the ground state is even; for example, for a 3 by 3 lattice with 3 holes, 3 by 4 with 2 or 4 holes, 3 by 5 with 3 holes. For number of holes other than two the energy is not a monotonic function of ϕ but the three main points above hold. They also hold for a 4 by 4 lattice with periodic boundary conditions, as is shown in Fig. 1, for the two values $\phi = 0, \pi$ where the statistics can be defined.

To amplify on our observation about the spin cascade for $J/t = 0$ we show in Table I numerical results for the ground-state spin density for different hole concentrations ρ as a function of the statistical phase ϕ. The lattices we consider are strips with 2 by N sites. We see that close to the bosonic point and for all hole densities the fully spin polarized state is stable, for small concentrations it is also stable at the fermionic point (Nagaoka's theorem) while it becomes unstable for larger fermionic hole concentrations. It is interesting to note a region of stability for large hole concentrations and intermediate statistical phases.

To start analyzing the influence of the spin background in the motion of the holes we consider next the simplest possible system that allows for two hole exchange and that can be solved analytically; a single square (2 by

2 sites plaquette) with two holes and two spins. The eigenvalues $\epsilon(S,k)$ of spin S and momentum k are given by

$$\varepsilon(0,0) = -J,$$

$$\varepsilon(0,\pi/2) = -J/2 \pm \sqrt{(J/2)^2 + 4[1-\sin(\phi/2)]t^2},$$

$$\varepsilon(0,\pi) = -J,$$

$$\varepsilon(0,3\pi/2) = -J/2 \pm \sqrt{(J/2)^2 + 4[1+\sin(\phi/2)]t^2};$$

$$\varepsilon(1,0) = \pm 2\sqrt{2}t\cos(\phi/4),$$

$$\varepsilon(1,\pi/2) = 0,$$

$$\varepsilon(1,\pi) = \pm 2\sqrt{2}t\sin(\phi/4),$$

$$\varepsilon(1,3\pi/2) = 0.$$

In Fig. 2 we show the energy of the lowest level in the singlet and triplet subspaces. The three main points mentioned above are also evident in this very simple system: for $J/t = 0$ the ground state is at $\phi = 0$ with S=1 (actually degenerate with the $\phi = \pi$ point S=0), while for $J/t > 0$ the singlet ground state has the lower energy with $\phi = \pi$. In this simple system it is clear that the presence of a singlet spin wave function leads to an apparent inversion of the hole statistics (if the relative energy is taken as criterion). To examine the possibility that the holes are just localized at the walls of the lattice and the results can easily be explained using the four-sites ring analysis, we show in Table II the average density for the different lattice sites of the 4 by 4 lattice with open boundary conditions, for $\phi = 0, \pi$ and various values of J/t. We find that for increasing J/t there is an increasing tendency for the holes to concentrate at the lattice walls but no sign of clumping till rather large J/t values. We also find that in agreement with our assignment of statistics the hole density is higher at the center of the cluster for $\phi = \pi$ than for $\phi = 0$ which is consistent to a bosonic behavior.

Finally one more remark can be relevant in this calculation; two fermions on a two-dimensional lattice with opposite spin and hard-core repulsion have the same energy as two hard-core bosons. It is possible then to argue that the two holes for $\phi = \pi$ (the nominal t-J model) ef-

TABLE I. Ground-state spin (normalized to maximum spin possible for given hole concentration) for different hole densities $\rho = M/2N$ (number of holes/total number of lattice sites) and different statistical phases ϕ. All the lattices are strips with 2 by N sites and open boundary conditions.

ρ \ ϕ	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
$\frac{12}{14}$	1	1	1	0	0	1	1	1	1	0	0
$\frac{10}{12}$	1	1	1	0	0	1	1	1	1	0	0
$\frac{8}{10}$	1	1	1	0	0	1	1	1	0	0	0
$\frac{6}{8}$	1	1	1	0	0	1	1	1	0	0	0
$\frac{10}{14}$	1	1	1	0	0	1	1	0	0	0	0
$\frac{8}{12}$	1	1	1	0	0	1	0	0	0	0	0
$\frac{6}{10}$	1	1	1	1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0
$\frac{8}{14}$	1	1	1	1	$\frac{1}{3}$	1	0	0	0	0	0
$\frac{6}{12}$	1	1	1	1	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	0	0
$\frac{4}{8}$	1	1	1	1	0	$\frac{1}{2}$	0	0	0	0	0
$\frac{6}{14}$	1	1	1	1	1	0	$\frac{1}{4}$	0	0	0	0
$\frac{4}{10}$	1	1	1	1	1	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0
$\frac{4}{12}$	1	1	1	1	1	1	0	0	0	$\frac{1}{2}$	$\frac{1}{2}$
$\frac{4}{14}$	1	1	1	1	1	1	1	1	0	$\frac{3}{5}$	$\frac{3}{5}$
$\frac{2}{8}$	1	1	1	1	1	1	1	1	0	0	0
$\frac{2}{10}$	1	1	1	1	1	1	1	1	1	1	1
$\frac{2}{12}$	1	1	1	1	1	1	1	1	1	1	1
$\frac{2}{14}$	1	1	1	1	1	1	1	1	1	1	1

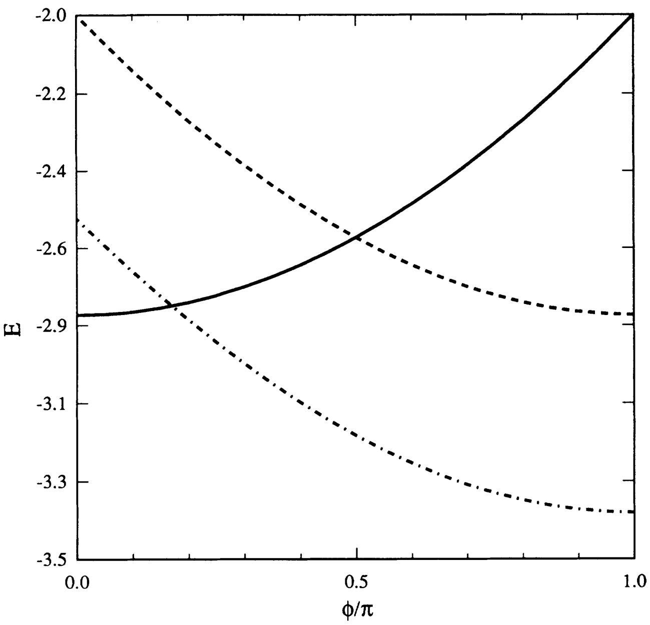

FIG. 2. Energy as a function of ϕ of the two lowest levels of the 2 by 2 plaquette with two holes. Solid line for S = 1, $k = 0$ (independent of J/t). Dashed for S = 0, $k = 3\pi/2$, $J/t = 0$, dot dashed for S = 0, $k = 3\pi/2$, $J/t = 1.0$.

fectively carry a spin and are bound to a singlet wave function.

III. ANALYTIC CALCULATIONS AND INTERPRETATION

The numerical calculations that we have performed indicate three inescapable conclusions; (i) in the absence of Heisenberg interactions the lowest energy is obtained from bosonic statistics. (ii) As the statistical phase is continuously varied toward fermionic statistics, there is usually a "spin cascade" from maximum to minimum total spin. (iii) When the Heisenberg interaction dominates, the lowest energy is achieved by fermionic statistics. We will verify some of these conclusions analytically, but before we do, we point out that the third conclusion is naively quite a surprise.

TABLE II. Hole density at the different lattice sites of the 4 by 4 lattice with open boundary conditions; d_1 denotes the four corner sites, d_2 the side sites, and d_3 the center sites.

		$\phi = 0$	$\phi = \pi$
	d_1	0.055	0.069
J/t=0.0	d_2	0.116	0.125
	d_3	0.213	0.181
	d_1	0.099	0.080
J/t=0.4	d_2	0.129	0.128
	d_3	0.141	0.165
	d_1	0.137	0.126
J/t=1.0	d_2	0.137	0.132
	d_3	0.067	0.111
	d_1	0.290	0.257
J/t=4.0	d_2	0.105	0.115
	d_3	0.002	0.013

It is generally believed, and we shall indeed later prove, that bosonic statistics make the most out of kinetic energy or hopping. At first sight, the inclusion of an additional term in the Hamiltonian which reverses this fact is not surprising, but upon closer inspection it can be seen that there is no direct dependence of the Heisenberg interaction on statistics (because holes do not move under the action of the Heisenberg term) and therefore any energy difference between two systems with different statistics must be directly attributable to their respective kinetic energies. The only conclusion that can be drawn, is that the presence of Heisenberg interactions can restrict the motion of bosons in comparison to the motion of fermions. Obviously it is the presence of the "spin bath" which leads to the change in motional characteristics, but this fact ought to be understood.

In order to develop a physical picture for the phenomenon that we are studying, we will now "over"-interpret the solution that we find for the single square with two holes (or equivalently two particles). The first point to observe is that our three conclusions remain basically intact for this example: In the absence of Heisenberg interactions bosonic statistics does indeed yield the absolute ground state. However, close inspection of the fermionic result reveals that there is another degenerate absolute ground state. A comparison of the spin wave function shows that the bosonic state has total spin one while the fermionic state has total spin zero. This is the remnant of the spin cascade for this small cluster. For nonzero Heisenberg interactions the fermionic state yields the ground state.

These results can be understood using the idea of transmutation of statistics. The spin wave function introduces new degrees of freedom into the system which can be used to alter the statistics of particles. When two parallel spin particles are exchanged, we find the usual statistical phase, but if we exchange two particles in a relative singlet, then we obtain an additional phase from the antisymmetry of the spin wave function. Two fermions in a spin singlet then exchange with a bosonic phase while two bosons in a spin singlet exchange with a fermionic phase. For the square, where we have only two particles and one permitted exchange, two fermions in a spin singlet behave precisely as two spinless hard-core bosons which explains the degeneracy found in this case of a single square. Obviously, for cases with more than two particles it is not possible to achieve singlet correlations between all particles simultaneously, and so in general the transmutation of statistics is not complete. Nevertheless, this idea does provide us with a physical overview to our results: In the absence of Heisenberg interactions, spinless hard-core bosons achieve the best possible kinetic energy. For bosonic statistics a ferromagnetic spin background maps the problem onto spinless hard-core bosons which then achieves this absolute bound. For fermions, a low spin state is stabilized. The probability that exchange between fermions in relative spin singlets is optimized and the system behaves as much like a spinless hard-core bose gas as the spin wave function will allow it to. When the Heisenberg interactions are switched on, the fermionic ground state, which has low spin correlations to promote singlet exchange, gains a huge energy while the ferromagnetic bosonic ground state gains nothing. Eventually the Heisenberg interactions become so strong that the ferromagnetism cannot survive, and there is a cascade down to a Heisenberg-dominated spin singlet. In this spin singlet, bosonic exchange will frequently occur in a relative spin singlet, and so the bosons will start to exchange fermionically which in turn will lead to a worse kinetic energy than the equivalent fermionic system.

So far we have treated the problem numerically on finite clusters and tried to interpret the solution using the toy model of the isolated square. In order to test our picture on the true infinite two-dimensional lattice, we have elected to perform some analytic calculations on the two cases of fermionic and bosonic statistics. Obviously the model is beyond the scope of our analytic tools in general, but there are two limits which are susceptible to partial analysis. The first limit is that of $J/t \to 0$, for which we will show that bosonic hole statistics always provides a lower kinetic energy than fermionic hole statistics, and the second limit is that of $t/J \to 0$, for which we show that fermionic hole statistics provides a lower kinetic energy than bosonic hole statistics.

Before we proceed to the mathematical analysis, we state one important interpretational consideration; the manner in which the statistics manifests itself in this problem is controlled solely by the kinetic energy. The Heisenberg interaction acts on frozen hole configurations and yields the same result independent of the hole statistics. It is only when the kinetic term permutes holes that the statistics shows up. In comparing energies in the presence of J/t, one is still comparing kinetic contributions.

Our analytic development employs an infrequently used representation for the state space; a form of spin-charge separation description:

$$|\Psi> = \sum_{i_1,i_2,\ldots,i_h} h^\dagger_{i_1} h^\dagger_{i_2} \cdots h^\dagger_{i_h} |0> \alpha_{i_1 i_2 \cdots i_h} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m} S^{\sigma_1\sigma_2\cdots\sigma_m}_{j_1 j_2 \cdots j_m} |\sigma_1 \sigma_2 \cdots \sigma_m>$$
$$\equiv \sum_{j_1,j_2,\ldots,j_m} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m} A^{\sigma_1\sigma_2\cdots\sigma_m}_{j_1 j_2\cdots j_m} c^\dagger_{j_1\sigma_1} c^\dagger_{j_2\sigma_2} \cdots c^\dagger_{j_m\sigma_m} |0> . \quad (2)$$

The states are separated into hole configurations, denoted by $h^\dagger_{i_1} h^\dagger_{i_2} \cdots h^\dagger_{i_h} |0>$ where $h^\dagger_i$ are assumed to be bosonic, with a positive definite amplitude of $\alpha_{i_1 i_2 \cdots i_h}$, combined with a collection of normalized wave functions, $S^{\sigma_1\sigma_2\cdots\sigma_m}_{j_1 j_2\cdots j_m}$, one for each spatial configuration of holes. All the phases have been extracted, both statistical and chemical bonding, and placed into this spin wave function. The labels $i_1 i_2 \cdots i_h$ denote the hole positions and the labels $j_1 j_2 \cdots j_m$ denote the particle positions. It is clear that a charge configuration can be uniquely defined by either the holes or the particles, and we have chosen to use holes as charges in order to be consistent with the majority of the published literature, even though the arguments are slightly complicated. The reason that we employ this representation should become apparent as we proceed, so we will only spend time developing an understanding of the action of the Hamiltonian in our chosen basis.

The Heisenberg exchange acts on the spin wave function leaving the holes fixed. In this representation the Heisenberg interaction is quite simple. The kinetic energy term is rather more complicated however, since it exchanges a hole with a particle and thereby connects to a spin wave function associated with a different hole configuration. The actual spin configuration is conserved by each individual hop, however. In order to clarify the picture it is worth writing down the Schrödinger equation for the case $J/t = 0$ in this representation:

$$E\alpha_{i_1 i_2\cdots i_h} S^{\sigma_1\sigma_2\cdots\sigma_m}_{j_1 j_2\cdots j_m} = -t \sum_p \sum_{<i_p j_q>} \alpha_{i_1 i_2 \cdots i_{p-1} j_q i_{p+1}\cdots i_h} S^{\sigma_1\sigma_2\cdots\sigma_{i_{q-1}}\sigma_{j_q}\sigma_{i_{q+1}}\cdots\sigma_m}_{j_1 j_2\cdots j_{q-1} i_p j_{q+1}\cdots j_m} , \quad (3)$$

which is valid for both fermions and bosons. The statistical phase is being controlled by the phase of the spin wave function in this representation, viz.,

$$S^{\sigma_1\sigma_2\cdots\sigma_p\cdots\sigma_q\cdots\sigma_m}_{j_1 j_2\cdots j_p\cdots j_q\cdots j_m} = \tau_s S^{\sigma_1\sigma_2\cdots\sigma_q\cdots\sigma_p\cdots\sigma_m}_{j_1 j_2\cdots j_q\cdots j_p\cdots j_m} , \quad (4)$$

where τ_s is the statistical phase, $\tau_s = +1$ for bosons, $\tau_s = -1$ for fermions.

In writing down our spin-charge separated basis, we have chosen a particular order for the sites in any fixed holes configuration. As the holes move around under the action of the Hamiltonian, we can arrive at the same hole configuration but with the holes in a different order. It is at this moment that the statistical phase plays a critical role, changing the phase of this contribution with respect to the original. In our representation, the interplay between the statistical phase and the spin configuration is the issue. When two particles are exchanged, their spins are simultaneously exchanged. The symmetry of the spin wave function under exchange now controls the effective statistics. Since if for fermions the spin wave function was totally antisymmetric, then this would compensate precisely for the statistical phase yielding bosonic statistics for the motion. The real physical issue is whether or not a spin configuration can be antisymmetric enough to have the same physics as the totally antisymmetric case.

The interpretation for this Schrödinger equation is simple, the spin wave function of a particular configuration is a weighted average of the spin wave functions associated with hole configurations connected to it by a single hop. Since the charge-wave function coefficients $\alpha_{i_1 i_2 \cdots i_h}$ are chosen to be positive definite, energy can only really be reduced if the spin configuration changes as the holes move about.

This fact allows us to show our first result, that hard-core bosons always have lower energy than fermions in the limit that $J/t = 0$. The first step is to observe that

$$E = -t \sum_{p} \sum_{<i_p j_q>} \alpha_{i_1 i_2 \cdots i_{p-1} i_p i_{p+1} \cdots i_h} \alpha_{i_1 i_2 \cdots i_{p-1} j_q i_{p+1} \cdots i_h} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_m} S^{\sigma_1 \sigma_2 \cdots \sigma_{q-1} \sigma_q \sigma_{q+1} \cdots \sigma_m}_{j_1 j_2 \cdots j_{q-1} i_p j_{q+1} \cdots j_m} S^{*\sigma_1 \sigma_2 \cdots \sigma_{q-1} \sigma_q \sigma_{q+1} \cdots \sigma_m}_{j_1 j_2 \cdots j_{q-1} j_q j_{q+1} \cdots j_m} \qquad (5)$$

and therefore in this representation we find a scalar product in spin space. For the Bose gas we can immediately deduce that the ground state is ferromagnetic. The argument will be used several times, so we will explain it once. If we have an eigenstate for which the spin configuration changes as a function of hole configuration, then we can construct a ferromagnetic state with a lower energy. The variational theorem then establishes that the ground state has a fixed spin configuration. We cannot prove that the ground state is ferromagnetic, as one hole in a lattice as in Fig. 3 has multiply degenerate solutions, but we can show that ferromagnetism yields a ground state. The variational state which proves the theorem is that where we use the same charge state, viz., the same values for $\alpha_{i_1 i_2 \cdots i_h}$, but a ferromagnetic spin state. The change in spin configuration yields a scalar product in spin space which is less than unity which in turn places the ferromagnetic state lower in energy.

We can use an almost identical argument to prove that the boson ground state is lower in energy than the fermion ground state. The charge state found in the fermion ground state yields a variational ferromagnetic boson state with lower kinetic energy. We note in passing that this argument will prove Nagaoka's theorem since statistics are irrelevant at the one-hole level in a saturated ferromagnet.

In the limit of vanishing J/t, ferromagnetic Bose states are always lower in energy than other states (including states with arbitrary ϕ, although we have not proved this directly). It is worth noting that we now have a generalization of Nagaoka's theorem to any hole concentration: For any hole concentration in the bosonic t-J model, with negative hopping matrix elements there is a ferromagnetic ground state. Obviously this result is not relevant to the fermionic model of physical interest, but the rigorous bound on the kinetic energy might prove of some use.

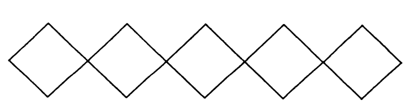

FIG. 3. A line of corner-sharing squares. The ground state of the t-J model in the limit $t/J \rightarrow 0$ finds isolated squares with four spins in a fluctuating Néel state. The Nagaoka state (one hole at $J = 0$) is also very degenerate for this geometry.

We now move on to the limit $J/t \rightarrow \infty$. Our representation is also quite useful in the limit $J/t \rightarrow \infty$, because in the absence of hopping the different hole configurations are unconnected. The eigenstates of the system may be chosen to have fixed hole configuration and also to have spin configurations which are eigenstates of the Heisenberg Hamiltonian restricted to bonds connecting atoms which are both occupied by particles. The analysis of the limit $J/t \rightarrow \infty$ then involves three elements: a derivation of the particular hole configuration which achieves the ground-state energy, a study of how degenerate perturbation theory might lift any residual degeneracy between different hole configurations yielding the same ground-state energy, and finally a calculation of the role of statistics in nondegenerate perturbation theory, and in particular which type of statistics are preferred and for what physical reason. Some of these issues are more difficult to treat than others, and we will briefly discuss each in turn.

The initial problem of finding the best hole configuration seems physically transparent and is expected to lead to "clustering" of charge. Two isolated holes break all of the bonds to their nearest neighbors whereas two neighboring holes avoid breaking the bond between them twice. A dense cluster of holes will then minimize the number of broken bonds and supposedly maximize the Heisenberg energy from the unbroken bonds. Unfortunately, although we believe this argument is usually correct, it can fail for rather subtle reasons. Although a dense cluster of holes ensures that the Heisenberg Hamiltonian has the maximum number of bonds to act on, there is no guarantee that all the bonds can be used efficiently. One might then expect a topologically frustrated counterexample, with a careful positioning of holes unfrustrating the geometry, e.g., that in Fig. 4 for which a ground state is obtained by pairing all electrons up into nearest-neighbor singlets which can be laid down at random, but in fact the real situation is much worse. Even bipartite geometries can fail, e.g., Fig. 3 for which isolated Néel squares obtain $-0.5J/t$ per particle whereas a concentrated region obtains only $-0.4847J/t$ per particle. For this case quantum fluctuations play a decisive

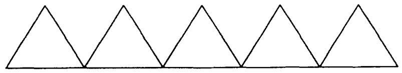

FIG. 4. The "sawtooth" geometry. The ground state of the t-J model as $t/J \rightarrow 0$ finds isolated pairs of spins in relative spin singlets in different triangles.

role. In this paper we will not pursue this problem but we will assume that the holes do "condense" into a single cluster, an eventuality that we believe to be relevant for the square lattice of present interest. The second issue is that of degeneracies between states with different hole configurations. There are two classes; trivial degeneracies, such as clusters related by periodicity and point group, and nontrivial degeneracies where the clusters are distinct shapes. We view this second class as being accidental and rare, and so we will ignore it, considering only trivial degeneracy. The degeneracy is broken to leading order by a sequence of hops which transform one cluster type into another.

The first point is that for a large cluster we must anticipate moving a large number of particles over long distances and so the contribution will be of very high order and unlikely to be relevant to the more important issue of which type of statistics are relatively stable. The second point is that the magnitudes of the matrix elements are independent of statistics and only the overall phase of the matrix element connecting different hole configurations depends on the statistics. For a bipartite geometry, although the particular **k**-point and point-group symmetries might be expected to depend on statistics, the total energy probably will not. For translational symmetry we would expect the lowest energy to be found at either zone center or zone boundary, with only an odd number of fermions being moved yielding a different **k** point. For point-group symmetry the particle permutation is more involved but the conclusion is similar.

Having suggested that the lifting of degeneracy is irrelevant, we are left to analyze which statistics have lower energy in normal perturbation theory. Obviously, the consequences of statistics can only be felt when particles are exchanged with each other. In practice, the first process that yields an energetic difference is the exchange of particles around the smallest loop, which is completed in precisely the same number of hops as the loop is long. As we are predominantly interested in the square lattice we will devote ourselves to this case only, although the basic ideas are applicable to any geometry. Exchange around squares will occur along the boundary of the cluster. At first glance we might anticipate having to consider squares with either one, two, or three particles present, but this proves not to be the case, since a cyclic permutation of an odd number of fermions yields the same statistical phase as a corresponding permutation of bosons. The degeneracy is broken solely by exchange of pairs of particles around squares, leading us back toward our initial square-toy calculation. Let us focus on one square with the knowledge that the final result is a sum over all contributions from all possible squares around the boundary. The physical effect which breaks the degeneracy is the fact that the spin wave function can transmute the statistics between fermions and bosons. Bosons prefer to exchange in a total spin triplet whereas fermions prefer to exchange in a total spin singlet. The two contributions turn out to be very easy to separate. Any spin configuration may be decomposed quite generally into two contributions for which a particular bond is either singlet or triplet. The projection operators $P_s^2 = P_s = \frac{1}{4} - \mathbf{S}_1 \cdot \mathbf{S}_2$ and $P_t^2 = P_t = \frac{3}{4} + \mathbf{S}_1 \cdot \mathbf{S}_2 = 1 - P_s$ accomplish this for the singlet and triplet contributions, respectively. For a particular exchange in a particular direction we obtain a perturbative energy of

$$E = -t\frac{1}{\epsilon_1 J}t\frac{1}{\epsilon_2 J}t\frac{1}{\epsilon_3 J}t[< P_t > - < P_s >]\sigma_s, \qquad (6)$$

where $\epsilon_1, \epsilon_2, \epsilon_3$ are the three Heisenberg energies for the intermediate spin configuration, σ_s is the statistical phase (viz., $\sigma_s = +1$ for bosons and $\sigma_s = -1$ for fermions), and $< P_s >, < P_t >$ are the probabilities that the particle pair which exchange are singlet and triplet, respectively. It is now clear which of the two statistics are relatively stable in which spin state. If the boundary of the cluster is predominantly triplet then bosons will be relatively stable, whereas if the boundary of the cluster is predominantly singlet then fermions will be relatively stable. For antiferromagnetic coupling we expect fermions to be relatively stable. Remember two facts: First that a Néel state finds equal probabilities of finding each bond singlet or triplet and quantum fluctuations increase the singlet probability, and second that singlet correlations are enhanced near the edge of a system because of the effective reduction in dimensionality and the resulting drop in the number of nearest neighbors competing for correlations. The final result we obtain has the form

$$\delta E = -\frac{t^4}{J^3} \sum_{\substack{\text{doubly} \\ \text{occupied squares}}} \sigma_s[< P_t > - < P_s >] \sum_{\text{routes}} \frac{1}{\epsilon_1 \epsilon_2 \epsilon_3}, \qquad (7)$$

where the sum over routes includes all possible intermediate states for exchanges in both directions. The result fails for two holes, where a degeneracy is reached at order t^2/J (viz., $\epsilon_2 = 0$) but we expect it to be valid for almost all other cluster types.

It is interesting to observe that this energy difference vanishes for a "classical" Néel state, and so the effect relies on the presence of quantum fluctuations. We believe that this observation is physically significant and can be used to indicate why the more exotic behavior has been observed in low-dimensional systems. Another physical consequence of the dependence of the effect on quantum fluctuations, is that if the spin interaction were Ising-like, then there would be no gain in energy from the fermionic case, because to leading order $< \rho_s > = < \rho_t > = \frac{1}{2}$ in the Ising ground state.

In summary, it is perfectly natural to use the idea that the spin system can transmute statistics in order to explain the behavior of our generalized t-J model. Fermions prefer low-spin correlations while bosons prefer high-spin correlations, since in each case they move locally like hard-core spinless bosons which rigorously optimize kinetic energy. We are not suggesting that the fermionic t-J model behaves at low temperature like a charged Bose gas, since the long-range correlations have never been seriously considered. We are suggesting that on a local level the way to optimize kinetic energy in a t-J model is to choose the spin wave function in such a way that as many particle exchanges as possible are performed with a bosonic phase. The consequences of this observation are not immediately clear, but might lead to faithful Bose descriptions.

IV. CONCLUSIONS

In this paper we have presented a way of demonstrating the effect of a spin environment on the motion of holes in a doped antiferromagnet by using as a probe the effect of additional statistical fluxes through the holes.

From our study we found that if the dependence of the ground-state energy on the statistics is taken as a criterion, then for $J/t > 0$, the fermionic holes in the original t-J model behave as hard-core spinless bosons. We could have chosen the opposite representation that of bosonic holes and fermionic spin; in that case the apparent inversion of statistics would have occurred for $J/t \simeq 0$. This observation indicates what might be a preferred representation of the hole and spin systems where they appear decoupled as far as the statistics is concerned; fermionic holes and bosonic spins for $J/t \simeq 0$ or bosonic holes and fermionic spins for $J/t > 0$.

Of course the dependence of the energy on the statistics of the hole system is in principle unrelated to the statistics of charged quasiparticles although the possible presence of a spin gap could make this connection more plausible. t-J models for which there is probably a spin gap can be written down,[7] and a study of the lowlying excitations suggests spinless hard-core excitations are present within the spin gap. Numerical studies of excitations are very difficult and are very much for the future.

We have proved an unremarkable theorem, that spinless hard-core bosons have lower kinetic energy than any other statistics of particles for the case of unfrustrated hopping. Of slightly more physical interest, is the numerical observation that for particles moving in the presence of low-spin correlations, fermionic statistics yields the lowest kinetic energy, since fermions mimic spinless hard-core bosons best on a local level for this case. In simple terms, if the most frequent exchange is that of a pair of particles in the confines of a single square, then a low-spin background favors fermionic statistics since two fermions in a singlet exchange in an identical fashion to two hard-core bosons.

To find more about the possibility of fractional statistics, the excitation spectrum must be studied, which we think is not feasible within this small cluster calculation as fractional statistics implies the existence of a broken symmetry certainly not present in a finite-size system. It is definitely necessary to extend these calculations to larger lattices and hole densities to examine if these conclusions are general.

Also from our analysis it became evident that the mechanism of phase separation is not purely due to a counting of broken antiferromagnetic bonds; due to the motion of the holes the phase separation is favored for fermionic holes (the nominal t-J model) compared to a one with bosonic holes.

Finally the suggestion of the bosonic behavior of holes for nonzero J/t is intriguing in the context of high-tempererature superconductivity.

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*Present address.

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