Large physical spin approach for strongly correlated electrons

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Abstract

We present a novel approach for a systematic large–spin expansion of the $t$-$J$ Hamiltonian which enables us to work without the constraint of no double occupancy. In our scheme we can perform the large–spin limit ensuring that the low energy spin excitations are in exact correspondence with the physical excitations of the $s = \frac{1}{2}$ Hilbert space. As a consequence, we expect a smooth dependence of the physical quantities on the expansion parameter $1/s$. As a first application of the method we study the case of a single hole in a Néel background. A systematic expansion in fluctuations about this stable solution indicates that by increasing $t/J$ the quasiparticle weight strongly depends on the momentum carried by the hole. Results, obtained on small lattice sizes, are found in excellent agreement with exact diagonalization data.

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The $t$-$J$ model in two spatial dimensions is perhaps the most challenging “unsolved” problem in the theory of strongly correlated electrons, since it is now commonly accepted to represent the low–energy Hamiltonian for the two dimensional copper–oxide high–temperature superconductors. Recent calculations based on the old fashioned, but reliable high–temperature expansion techniques, have indicated that spin–charge separation, obviously present in this model in one dimension, may also characterize the elementary excitations in 2D, leading to a break-down of Fermi liquid theory and to a possible explanation of the anomalous properties of the high–temperature superconductors. [1]

We consider $N_h$ holes interacting by the $t$-$J$ Hamiltonian

$$H_{tJ} = -t \sum_{\langle i,j \rangle, \sigma} P(c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) P + J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} N_i N_j),$$

where $\langle i, j \rangle$ denotes a summation over the nearest neighbor (n.-n.) sites of the lattice, $P$ is the projector onto the Hilbert space without doubly occupied sites, $\vec{S}_i$ and $N_i$ are the spin and number operators at site $i$, and $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ are the usual creation and annihilation operators for electrons of spin $\sigma$. Henceforth we assume $t \geq 0$, $J \geq 0$.

Due to the difficulty to deal with the projector of no double occupancy, several semi-classical approaches [2–5] leading to a mean–field description of $H_{tJ}$ have been proposed. In particular, in the large–spin approaches presented so far, the simplification of the $t$-$J$ Hamiltonian is achieved by generalizing the spin-$\frac{1}{2}$ polarization state of the electron to an arbitrary spin $s$ state and by giving a fictitious spin $(s - \frac{1}{2})$ to the hole. The various methods differ for the definition of the enlarged Hamiltonian, a freedom left by the very fact that in a large–spin generalization one can only require that the physical Hilbert space, as well as the $t$-$J$ model $H_{t,J}$, must be recovered for the value $s = \frac{1}{2}$ of the expansion parameter. Unfortunately, all of them face the following fundamental difficulty: as soon as the extended Hilbert space is larger than the physical one, spurious low–energy elementary excitations emerge. Hence, it is not at all guaranteed that the low–lying excitations of the extended Hamiltonian correspond to some physical excitation of the original one, so that it becomes difficult or even impossible to derive reliable results by performing a systematic expansion.
in fluctuations about the mean–field obtained by letting $s \to \infty$.

Explicitly, in the Kane et al. model one obtains the Néel background as the mean–field solution for small $J/t$, but for $s > \frac{1}{2}$ some of the allowed excitations change the spin of the hole, which is clearly unphysical. Other large–spin generalizations instead face the problem that the hole propagation becomes a nonperturbative process in the $1/s$ expansion. In the latter case, as was shown by two of us in Ref. [6], one obtains phase separation even at small $J/t$, whereas it is now believed that the uniform ground–state is stable in the physical sector [7,8].

In this work we propose a new method to simplify at large spin the $t$-$J$ model without facing the previous difficulties. In our approach we do not deal directly with $H_{tJ}$, but consider instead a natural extension of it as introduced by Sutherland [9], because the latter allows us to apply the spin–wave theory with a one–to–one correspondence with the physical excitations.

In the $t$-$J$ Hamiltonian the single site $i$ can be occupied by 3 kinds of “objects”: A hole (boson) $|0\rangle_i$, an electron of spin-up $|\uparrow\rangle_i = c_{i,\uparrow}^\dagger |0\rangle_i$, and an electron of spin-down $|\downarrow\rangle_i = c_{i,\downarrow}^\dagger |0\rangle_i$ (fermions) whereas, apart for an irrelevant energy shift, $H_{tJ}$ can be thought of as the operator permuting pairs of n.-n. objects, with weight $t$ for permutations of objects of opposite statistics, and weight $J/2$ ($-J/2$) for permutations of fermions (bosons). In order to work without the local constraint of no doubly occupancy, we consider the extended Hamiltonian $H$ acting on objects of two fermion and two boson species by permutation of pairs of neighboring objects with the same weights as in the $t$-$J$ model. Because the number of objects of a given species is conserved by construction, the reduction to the physical model can be obtained by projecting onto the invariant subspace where one boson species is absent. Hence, in our approach the projector operator $P$ is washed out, as for the projection amounts just to fix a conserved quantity.

To represent the extended Hamiltonian $H$ in a way suited for our developments, we denote the fermion and boson objects at site $i$ with the symbols $|1\sigma\rangle$ and $|0\sigma\rangle$ ($\sigma = \uparrow, \downarrow$), respectively, and use the representation $|0 \uparrow\rangle_i = f_i^\dagger |v\rangle$, $|1 \uparrow\rangle_i = |v\rangle$, $|0 \downarrow\rangle_i = f_i^\dagger Q_i |v\rangle$, $|1 \downarrow\rangle_i = f_i^\dagger Q_i^\dagger |v\rangle$. 


\[ |1\downarrow\rangle_i = Q_{i,-}|v\rangle, \] where \( f_i^\dagger \) and \( Q_{i,-} \) are a spinless fermion creation operator and a spin-\( \frac{1}{2} \) lowering operator, respectively. The extended Hamiltonian reads

\[
H = \sum_{\langle i,j \rangle} \left[ -t (f_i f_j^\dagger + f_j f_i^\dagger) \chi_{i,j} + \frac{J}{2} (1 - n_i - n_j) (\chi_{i,j} - 1) \right],
\]

where \( \chi_{i,j} = 2 \vec{Q}_i \vec{Q}_j + \frac{1}{2} \) and \( n_i = f_i^\dagger f_i \). A noticeable feature of the proposed model \( H \), to be contrasted with the case of \( H_{tJ} \) in a slave–fermion representation \([5,6]\), is the presence of the permutator operator \( \chi_{i,j} \) both in the magnetic and kinetic part, as well as the bilinear dependence on the fermion operators.

Henceforth we preserve the name of electron and hole for the two “particles” \(|1\sigma\rangle\) and \(|0\sigma\rangle\), respectively, and introduce the two commuting vector operators satisfying the algebra of the angular momentum

\[
\vec{S} = \sum_i (1 - n_i) \vec{Q}_i, \quad \vec{L} = \sum_i n_i \vec{Q}_i, \tag{1}
\]

The operators \( \vec{S} \) and \( \vec{L} \) act nontrivially on \(|1\sigma\rangle\) and \(|0\sigma\rangle\), respectively, and accordingly \( \vec{S} \) will be referred to as the physical spin and \( \vec{L} \) as the pseudospin. The analogy with the properties of the spin and pseudospin operators is not only formal and will be discussed elsewhere \([10]\). In the following we shall also refer to \( \vec{Q} = \vec{L} + \vec{S} \) as the isospin vector. The operators \([\] \) commute with \( H \), so that the quantum numbers spin \( S_z \), total spin \( S \), and pseudospin \( L_z \), total pseudospin \( L \) associated to both “particles” are conserved. The physical Hilbert space of \( H_{tJ} \) corresponds to the sector where the pseudospin attains its maximum value \( L_z = L = N_h/2 \).

Sutherland \([9]\) has shown quite generally that the ground–state of the Hamiltonian \( (H) \) is at most degenerate with the physical one with maximum pseudospin \( L_z \). Unfortunately, this statement is rigorously valid only in one dimension, and for the case of a single hole in any dimension. The latter case is of course trivial, because for one hole the pseudospin is by definition equal to the maximum value \( L = \frac{1}{2} \). The proof presented in Ref. \([9]\) is not valid in 2D. In fact, following the reasoning one would obtain that for \( J = 0 \) the ground–state
of $H_{i,j}$ is the fully polarized Nagaoka state, whereas it is known that for large doping the singlet Gutzwiller projected Fermi gas has macroscopically lower energy \[11\].

However, the Sutherland’s result is true for the special case $t = 0$ and probably remains valid for physically acceptable $J/t > 0$ in $D \geq 2$. Hence, we shall leave it as a “conjecture”. The importance of this conjecture is easily understood by noting that whenever it is satisfied, one can evaluate ground–state properties avoiding even the projection onto the $L_z = N_h/2$ sector.

The Hamiltonian $H$ still represents a highly nontrivial problem and we now consider the large–spin approach allowing to simplify the model. Noting that $\vec{Q}$ is a irreducible spin-$\frac{1}{2}$ operator, we consider arbitrary higher–dimensional representations of the isospin vector and define the enlarged Hamiltonian $H_s$ by substituting in the extended Hamiltonian $H$ the permutator operator $\chi_{i,j}$ with the rotationally invariant expression

\[
\chi_{i,j} \rightarrow \chi_{i,j}^{(s)} = \frac{1}{2s^2} \vec{Q}_i \cdot \vec{Q}_j + \frac{1}{2}.
\]

The overall factors and constants – irrelevant in the undoped case – are set by the requirement that $\langle \chi_{i,j}^{(s)} \rangle$ is one or zero if the isospins of the particles at sites $i,j$ are parallel or antiparallel, respectively. In our approach the Hilbert space is generalized by giving a fictitious spin-$s$ both to the electron (i.e., $|1\sigma\rangle$) and to the hole (i.e., $|0\sigma\rangle$) and in this respect it is quite different from the large–spin approaches proposed so far.

Because at zero doping isospin and physical spin coincide ($\vec{L} = 0$), our approach leads to the conventional spin wave–expansion for the Heisenberg antiferromagnet: The ground–state is a singlet and the physical spin–wave excitations have $S = 1$, i.e., they are independent of the magnitude of the spin $s$ of the extended Hilbert space. We see that in the large–spin limit the Hilbert space at each single site grows with $s$ but the low–energy excitations remain in one–to–one correspondence with those of the physical $s = \frac{1}{2}$ Hilbert space. We believe that this is the basic reason why the spin–wave expansion is so accurate for the undoped system and why $1/s$ is a smooth parameter and actually small \[12][14\].

At nonzero doping, for $s > \frac{1}{2}$ the observable (1) are no more conserved, unless for $t = 0$. 

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However the Hamiltonian $H_s$ always commutes with the isospin and it is therefore convenient to work in the subspace with $Q$ and $Q_z$ fixed. If for the original $t$-$J$ Hamiltonian the physical spin attains its minimum value - as it is expected for $J$ not too small – the Hilbert space with minimum $S$ and fixed $S_z$ is exactly equivalent to the one with $Q = [N_h/2]$ and say $Q_z = 0$ (for $N_h$ odd one has $S = 1/2$ as the minimum value). Hence, if we are able to classify the elementary excitations for $s \to \infty$ in the sector where $L$ is frozen to its maximum value, the same classification would hold in the physical Hilbert space, provided that there is no phase transition as a function of $1/s$.

In order to show that our $1/s$ expansion is the natural extension of the spin–wave theory even in the doped case, we focus our attention to the simplest possible nontrivial doping, i.e., when there is only one hole ($N_h = 1$) in a lattice of $M$ sites with periodic boundary conditions.

For large $s$ and $J$ not too small the stable semiclassical solution corresponds to a Néel background where the single hole can propagate with given momentum either on the $A$ or on the $B$ sublattice. Fluctuations over this semiclassical solution are obtained in the usual way by introducing boson operators $a_i^\dagger \approx \frac{Q_i}{\sqrt{2s}}$ if $i \in A$ ($\frac{Q_i}{\sqrt{2s}}$ if $i \in B$) that create a spin fluctuation over the Néel classical state $|N\rangle$. Thus a systematic expansion of the operator $\chi^{(s)}_{i,j}$ in $1/s$ is possible and we get

$$\chi^{(s)}_{i,j} = \frac{1}{2s}(\psi_{i,j}^\dagger \psi_{i,j} - 1) + O\left(\frac{1}{s^2}\right),$$

(3)

where $\psi_{i,j} = a_i^\dagger + a_j$. By replacing the expression (3) in the Hamiltonian $H$, both in the kinetic and the magnetic term, we then obtain an effective Hamiltonian for the single hole, which is characterized by a kinetic term coupling two boson and two fermion operators

$$\frac{1}{2s}(f_i^\dagger f_j^\dagger + \text{h.c.})[(a_i^\dagger + a_j)(a_i + a_j^\dagger) - 1].$$

Hence, it is remarkably different from the Kane et al. Hamiltonian, where instead the hole propagates by emitting or absorbing a single spin fluctuation. In our approach the spin is carried only by the boson $a_i^\dagger$ (which changes the spin by one), so that the conservation of $Q_z$ necessarily implies a quadratic Hamiltonian in the boson operators. A further simplification of $H_s$ can be obtained following Ref. [15,16].
for a different but similar problem. One can exactly trace out the single fermion $f_i^\dagger$ from the Hamiltonian $H$ using translation invariance and thus obtaining an effective spin Hamiltonian defined by the translation operator $T_{\tau \mu} a_i T_{-\tau \mu} = a_{i+\tau \mu}$ of spin–waves for nearest neighbour displacements $\tau \mu$

$$H_{\text{eff}} = \frac{1}{4s} \sum_{\tau \mu} (\psi_{0,\tau \mu}^\dagger \psi_{0,\tau \mu} - 1)(2t T_{\tau \mu} e^{i p \tau \mu} - J) + H_{SW},$$

(4)

where $i = 0$ denotes the origin and $H_{SW}$ is the Heisenberg Hamiltonian that, at first order in $1/s$ reads:

$$H_{SW} = \frac{1}{4s} \sum_{i,j} (\psi_{i,j}^\dagger \psi_{i,j} - 1).$$

Contrary to the undoped case, the Hamiltonian $H_{\text{eff}}$ cannot be solved analytically unless for the case $t = 0$, where $H_{\text{eff}}$ becomes quadratic \[17,15\]. However, a very good variational wavefunction that is exact in this limit, and which preserves all the symmetries of the Hamiltonian, is very easy to write down, in the form of the most general ground–state of a quadratic Bogoliubov Hamiltonian:

$$|\Psi_h\rangle = \exp\left\{\frac{1}{2} \sum_{i,j} B_{i,j} a_i^\dagger a_j^\dagger\right\} |N\rangle.$$  

(5)

$B_{i,j}$ is non zero only if $i$ and $j$ belong to different sublattices (to fulfil $Q_z = 0$) and its Fourier transform does not contain the modes at $k = (0,0)$ and $k = (\pi, \pi)$ (to fulfil $Q = 0$) \[8\]. In order to evaluate and then minimize the expectation value of the Hamiltonian $H_{\text{eff}}$ over the state (5), one needs to evaluate both the average $\langle \Psi_h | \psi_{i,j}^\dagger \psi_{i,j} | \Psi_h \rangle$, and the average of the quadratic form $\psi_{i,j}^\dagger \psi_{i,j}$ over $|\Psi_h\rangle$ and the state $|\Psi_h^\mu\rangle = T_{\tau \mu} |\Psi_h\rangle$ generated by the translation operator entering the kinetic term, i.e., $\langle \Psi_h | \psi_{i,j}^\dagger \psi_{i,j} | \Psi_h^\mu \rangle$. The state $|\Psi_h^\mu\rangle$ is clearly obtained by replacing in Eq. (5) the matrix $B_{i,j}$ with $B_{i,j}^\mu = B_{i,-\tau \mu,j-\tau \mu}$ and because both the states $|\Psi_h^\mu\rangle$ and $|\Psi_h\rangle$ are gaussian, it is then possible to evaluate the averages in closed form. In fact, given two gaussian states $|\Psi_A\rangle$ and $|\Psi_C\rangle$ of the form (3), with $A$ and $C$ the corresponding matrices entering the exponential, we have

$$\frac{\langle \Psi_A | a_i a_j^\dagger | \Psi_C \rangle}{\langle \Psi_A | \Psi_C \rangle} = G_{i,j}$$

$$\frac{\langle \Psi_A | a_i^\dagger a_j^\dagger | \Psi_C \rangle}{\langle \Psi_A | \Psi_C \rangle} = [A^* G]_{i,j}$$
\[
\frac{\langle \Psi_A | a_i a_j | \Psi_C \rangle}{\langle \Psi_A | \Psi_C \rangle} = [GC]_{i,j}
\]

where

\[
G_{i,j} = \frac{\langle \Psi_A | \Psi_C \rangle}{\langle \Psi_A | \Psi_A \rangle} \left[ (I - CA^*)^{-1} \right]_{i,j}
\]

\[
\langle \Psi_A | \Psi_C \rangle = \det^{-1/2} (I - CA^*)
\]

Using the above equations is it easy to work out an explicit expression for the expectation value of the Hamiltonian by simple linear algebra operations over the symmetric complex matrix \( B_{i,j} \). We have then obtained the optimal matrix \( B_{i,j} \) by minimizing the energy of the effective Hamiltonian \( H_{\text{eff}} \) with the standard conjugate gradient technique.

In table I we show data for the one hole energy (referenced to the undoped energy) and the quasiparticle weight \( Z = |\langle \Psi_H | \Psi_h \rangle|^2 \), where \( |\Psi_H \rangle \) is the ground–state of \( H_{SW} \). Because \( |\Psi_H \rangle \) is easily written in the gaussian form \( |H \rangle \) \( \text{[4,8]} \), Eq. (6) allows to evaluate \( Z \) straightforwardly. The agreement of the spin–wave estimates with the exact diagonalization results \( \text{[18]} \) is surprisingly good, yielding a robust evidence of a finite value for \( Z \) in the static \( t = 0 \) limit.

The accuracy of the method remains very good even for \( t > 0 \), as it is shown in Fig.1 for the quasiparticle weight at \( p = (0,0) \) and \( p = (\pi,\pi) \). We also see in Fig.1 (b) a clear transition of the quasiparticle weight for the \( (\pi,\pi) \) momentum. Its value changes of about two order of magnitudes also in the exact diagonalization data.

Our spin–wave approximation agrees with the exact diagonalization even in the details for \( t/J < 1 \). In fact, at the value \( t/J \approx 0.5 \), where in our simulation we find a singular point [see Fig.1 (b)], there is a true level crossing in the exact diagonalization. The true ground–state is actually orthogonal (with different symmetry) to \( |\Psi_H \rangle \). For larger \( t/J \) our approximate solution predicts that \( Z_{(\pi,\pi)} \) vanishes at a critical point for any finite size \( M \). At the moment a similar analysis \( \text{[19]} \) for momenta close to \( (\frac{\pi}{2},\frac{\pi}{2}) \) (which is found to be always the ground–state for \( M \to \infty \), consistent with the general believe in the physical
region $J$ not too small) indicates that $Z_{(\frac{\pi}{2}, \frac{\pi}{2})}$ remains finite up to $t/J \simeq 3$ \cite{15}. However we cannot exclude a transition to $Z_{(\frac{\pi}{2}, \frac{\pi}{2})} = 0$ at larger values of $t/J$ where our variational approach becomes unreliable.

The fact that some of the low energy excitations of the Mott insulator may have a "non trivial" character may lead to a completely new classification of the charge excitations in the low doping regime. This surely requires further analysis and more analytical work. For the time being we point that a drastic change of the weight for momenta differing by the nesting wavevector $q_\pi = (\pi, \pi)$, which are degenerate in energy, is a remarkable prediction of our approach which explains very well the numerical data on small systems and can be easily detected experimentally by photoemission experiments. For instance it is not possible to obtain the above property within the Kane et al. approach, because in this case the Green’s function satisfies to $G(k + q_\pi, \omega) = G(k, \omega)$, so that the weights $Z_k$ and $Z_{k+q_\pi}$ can only be equal.

Work is in progress for extending the calculation at finite density of holes and/or at smaller values of $J/t$.

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TABLES

TABLE I. Linear spin-wave estimates of the quasiparticle weights and the one-hole energies in the static limit \((t = 0)\) for the various clusters. The percentage relative errors refer to the spin-wave data as compared to the exact diagonalization results.

| M | QP Weight | % Error | Energy | %Error |
|---|-----------|---------|--------|--------|
| 8 | 1         | 0.0     | 2.5    | 0.0    |
| 10| 0.9919    | 0.0047  | 2.4308 | -0.35  |
| 16| 0.9724    | -0.22   | 2.3271 | -0.61  |
| 18| 0.9688    | 0.055   | 2.3052 | -0.60  |
| 20| 0.9637    | 0.050   | 2.2908 | -0.65  |
| 26| 0.9512    | 0.077   | 2.2609 |
| 32| 0.9422    |         | 2.2415 |
| ∞ | 0.820     |         | 2.17   |
FIGURES

FIG. 1.  (a) Quasiparticle weight as a function of $t/J$. The empty dots correspond to our spin–wave results; the full dots are the exact results on finite lattices. Continuous lines are guide to the eyes. (b) Same notation as in (a) except that the empty dots refer to the 100 sites lattice. The dotted line is a local unstable minima for $t/J > 0.6$