Supersymmetry in models with strong on-site Coulomb repulsion
- application to t-J model

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Abstract

A supersymmetric way of imposing the constraint of no double occupancy in models with strong on-site Coulomb repulsion is presented in this paper. In this formulation the physical operators in the constrained Hilbert space are invariant under local unitary transformations mixing boson and fermion representations. As an illustration the formulation is applied to the $t - J$ model. The model is studied in the mean-field level in the $J = 0$ limit where we show how both the slave-boson and slave-fermion formulations are included naturally in the present approach and how further results beyond both approaches are obtained.

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The $t - J$ model has become a focus in the study of strongly correlated metals and High-$T_c$ superconductors since it was proposed in late eighties [1]. Because of lack of small parameters for expansion, analytical understandings of the model were largely depending on mean-field theories which treat the constraint of no double occupancy only on average. So far, the most successful mean-field approaches to the $t - J$ model seems to be based on either the slave-fermion mean-field theory (SFMFT) [3] which is successful at very small doping when antiferromagnetic correlation is important, and the slave-boson mean-field theory (SBMFT) [2] which is successful at larger value of doping when the system becomes superconducting. The only difference between the two approaches is that two different representations of spin and electron operators are used to impose the constraint of no double occupancy. More recently, the focus in the study of High-$T_c$ superconductors has turned to the underdoped and spin-glass regimes where it is believed that the subtle interplay between antiferromagnetism and superconductivity determines the properties of this crossover region. In particular, the importance of $SU(2)$ symmetry in the underdoped regime of the $t - J$ model has been pointed out [4,5]. Alternatively, it was also suggested that an $SO(5)$ symmetry may play an important role in determining the competition between antiferromagnetism and superconductivity in the high-$T_c$ cuprates [6].

To understand the complicated behaviour in this regime of the $t - J$ model, it seems that a unified approach which incorporate both the advantages of the slave-fermion mean-field theory and the slave-boson mean-field theory is essential. In this paper, we shall show that it is possible in general to formulate models with constraint of no double occupancy in a way which incorporates the advantages of both slave-fermion and slave-boson representations. In this new formulation the physical operators are supersymmetric and are invariant under unitary transformations mixing fermion and boson representations. The formulation suggests that supersymmetry exists naturally in strongly-correlated systems where on-site Coulomb repulsions are strong. In the following, we shall use the $t - J$ model as an example to illustrate our approach. To begin with, we first consider the Hilbert space of a lattice model with constraint of no double occupancy imposed.
The constraint of no double occupancy implies that there are three possible states on any single lattice site in the model. The site can be either empty (hole state), or can be occupied by either an up- or down- spin electron. In the slave-boson approach, the hole state is represented as a boson, whereas spins are represented as fermions [2]. It is also equally valid to represent spins as bosons, and holes as slave fermions, as in the slave fermion treatment [3]. In our formulation we shall consider an enlarged Hilbert space where both possibility of representing hole and spins coexist as different states of the system, i.e. there are now six possible states per site in the Hilbert space, represented by

\[ |\sigma_i^{(f)}\rangle = c_{i\sigma}^+ |0\rangle, \quad |h_i^{(b)}\rangle = b_i^+ |0\rangle, \quad (1a) \]

and

\[ |\sigma_i^{(b)}\rangle = \bar{Z}_{i\sigma} |0\rangle, \quad |h_i^{(f)}\rangle = f_i^+ |0\rangle, \quad (1b) \]

where \( \sigma = \uparrow, \downarrow, c_{i\sigma}^+ \) and \( \bar{Z}_{i\sigma} \) are fermionic and bosonic spin creation operators, respectively and \( |0\rangle \) is the vacuum state. Similarly, \( b_i^+ \) and \( f_i^+ \) are bosonic and fermionic hole creation operators, respectively. Notice that we have seperated the states into "slave-boson" (1a) and "slave-fermion" (1b) groups in Eq. (1). For a system of \( N \)-lattice sites, both groups of states are allowed at all sites in our formulation and the total Hilbert space is thus \( 2^N \) times larger than the Hilbert space of the original model. The essence of our approach is to construct a Hamiltonian which is equivalent to the original model in all these \( 2^N \) groups of states, and consequently our system with enlarged Hilbert space is equivalent to \( 2^N \) replicas of the original model. To see how this Hamiltonian can be constructed for the \( t - J \) model we first consider spin operators.

We consider the spin operator \( \vec{s}_i \) at site \( i \),

\[ \vec{s}_i = \vec{s}_i^{(f)} + \vec{s}_i^{(b)}, \quad (2a) \]

where

\[ \vec{s}_i^{(f(b))} = \left( c^+(\vec{Z})_{i\uparrow}, c^+(\vec{Z})_{i\downarrow} \right) \vec{\sigma} \begin{pmatrix} c(Z)_{i\uparrow} \\ c(Z)_{i\downarrow} \end{pmatrix}, \quad (2b) \]
and $\sigma$ is the usual Pauli matrix. Notice that $\vec{s}^{(f)}$ and $\vec{s}^{(b)}$ are the spin operators in usual slave-boson and slave-fermion representations, respectively. It is obvious that $\vec{s}_i$ is itself a spin operator since it is the sum of two spin operators. The matrix elements $<\sigma^{(\alpha)}_i|\vec{s}_i|\sigma^{(\beta)}_i>$ where $\alpha, \beta = f, b$ and $\sigma, \sigma' = \uparrow, \downarrow$ can be computed easily where it is easy to see that $<\sigma^{(f)}_i|\vec{s}_i|\sigma^{(f)}_i> = <\sigma^{(b)}_i|\vec{s}_i|\sigma^{(b)}_i>$ and gives the usual spin operator matrix elements between spin-1/2 states whereas all other matrix elements with $\alpha \neq \beta$ are equal to zero. Thus the states $|\sigma^{(f)}_i>$ and $|\sigma^{(b)}_i>$ together form two identical replicas of spin-1/2 states on site $i$ with our definition of spin operator (2). It can then be shown by direct evaluation that the Hamiltonian

$$H_J = J \sum_{<i,j>} \vec{s}_i \cdot \vec{s}_j,$$

represents $2^N$ identical copies of Heisenberg interaction in our system of enlarged Hilbert space.

The electron annihilation and creation operators in our system can be defined as $\psi_{i\sigma} = h^+_i \xi_{i\sigma}$, and $\bar{\psi}_{i\sigma} = \xi^+_i h_i$, respectively, where

$$h_i = \begin{pmatrix} f_i \\ b_i \end{pmatrix}, \quad \xi_{i\sigma} = \begin{pmatrix} Z_{i\sigma} \\ c_{i\sigma} \end{pmatrix},$$

are doublets of hole and spin operators carrying fermion and boson statistics. It is straightforward to show that the electron operators defined this way satisfies the usual electron commutation relations in the Hilbert space spanned by Eq. (1). The kinetic energy term $H_t$ of the $t-J$ model can be constructed by requiring that the hopping matrix elements $<\sigma^{\alpha'}_j, h_i^{\beta'} | H_t | h_j^{\alpha}, \sigma^{\beta}_i >= -t_{ij} \delta_{\alpha \alpha'} \delta_{\beta \beta'}$, where $\alpha, \alpha', \beta, \beta' = b, f$ and $|h_j^{\alpha}, \sigma^{\beta}>$ represents a state with a hole belonging to group $\alpha$ on site $j$ and a spin $\sigma$ belonging to group $\beta$ on site $i$. Notice that the group indices $\alpha, \beta$’s are ”conserved” in constructing $H_t$. It is straightforward to show that

$$H_t = -t \sum_{<i,j>,\sigma} \left( c_{i\sigma}^+ b_j^+ c_{i\sigma} + c_{j\sigma}^+ b_j^+ f_i^+ Z_{i\sigma} + \bar{Z}_{j\sigma} f_j^+ b_i^+ c_{i\sigma} - \bar{Z}_{j\sigma} f_j f_i^+ Z_{i\sigma} + c.c. \right),$$

(4)
where we have considered a Hamiltonian with nearest neighbor hopping only. The four different terms in $H_t$ give the matrix elements of the hopping term between the four possible combination of groups of states at sites $<i,j>$. With this it is easy to verify that our system with Hamiltonian $H = H_J + H_t$ is equivalent to $2^N$ copies of the usual $t-J$ model.

Notice that the hopping term cannot be simply represented as $H_t = -t \sum (\psi^+_i \psi^i_{j\sigma} + c.c.)$ because of the sign difference in the "slave-fermion" term $\bar{Z}_{i\sigma}f_j f_i^+ Z_{i\sigma}$. This sign difference is well known in studies of slave-fermion mean-field theory [3].

The invariance of our system under change of group of states defined in Eq. (1) at any lattice site can be expressed in the language of supersymmetry. To see that first we note that the spin operator (2) can be written using the $\xi_\sigma$ fields as

$$ s^z_i = \frac{1}{2} (\xi^+_{i\uparrow} \xi_{i\downarrow} + \xi^+_{i\downarrow} \xi_{i\uparrow}), \quad s^+_i = \xi^+_{i\uparrow} \xi_{i\downarrow}, \quad s^-_i = \xi^+_{i\downarrow} \xi_{i\uparrow}, \tag{5} $$

where $\xi^{+}_{ia\sigma} = \bar{Z}_{ia} Z_{ia\sigma} + c^+_{ia\sigma}$. It is now easy to see that the spin and electron operators are invariant under the super-unitary transformation

$$ \xi_{i\sigma} \rightarrow U_i \xi_{i\sigma}, \quad h_i \rightarrow U_i h_i \tag{6} $$

where $U_i$’s are local $2 \times 2$ unitary super-matrices mixing the fermion and boson representations of spins and holes. The generators of the super-unitary transformations are superspin operators

$$ S^z_i = \frac{1}{2} \left( \sum_{\sigma} c^+_{i\sigma} c_{i\sigma} + b^+_i b_i \right) - \left( \sum_{\sigma} \bar{Z}_{i\sigma} Z_{i\sigma} + f^+_i f_i \right), \tag{7} $$

$$ S^+_i = \sum_{\sigma} c^+_{i\sigma} Z_{i\sigma} - b^+_i f_i, $$

$$ S^-_i = \sum_{\sigma} \bar{Z}_{i\sigma} c_{i\sigma} - f^+_i b_i, $$

where we also define the (magnitude)$^2$ of the superspin as $S^2 = S^z S^z + \frac{1}{2} (S^+ S^- + S^- S^+)$. Using the fact that the allowed states in our Hilbert space can only be singly occupied by either spin or hole, it is easy to show that

$$ S^2_i = \frac{3}{4} \left( \sum_{\sigma} \xi^+_{i\sigma} \xi_{i\sigma} + h^+_i h_i \right) = \frac{3}{4}. \tag{8} $$
where we have used the requirement that \( \sum \sigma (Z_{i\sigma}Z_{i\sigma} + c_{i\sigma}^+c_{i\sigma}) + f_i^+f_i + b_i^+b_i = 1 \) in our Hilbert space (1) in writing down the last equality. Notice that the constraint of no double occupancy is equivalent to the condition that the magnitudes of the superspins are fixed (= 1/2) on all lattice sites! In terms of the superspin operators, the slave-boson and slave-fermion representations are equivalent to fixing the direction of superspins to be pointing up and down, respectively and supersymmetry expresses the fact that the physical observables in the system are in fact, invariant under local (but time-independent) rotations in the superspin space. Notice that because of the "minus" sign in the "slave-fermion" hopping term \( \bar{Z}_{j\sigma}f_jf_i^+Z_{i\sigma} \), supersymmetry is straightly speaking, broken by the \( t-J \) term in the \( t-J \) model. However, our formulation of \( t-J \) model in the enlarged Hilbert space (1) does not require supersymmetry in the Hamiltonian and is still valid.

The Lagrangian of the \( t-J \) model in the enlarged Hilbert space is

\[
L = i\hbar \sum_{i,\sigma} \xi_{i\sigma}^+ \frac{\partial}{\partial t} \xi_{i\sigma} + i\hbar \sum_i h_i^+ \frac{\partial}{\partial t} h_i - H_t - H_J
\]

\[
+ \sum_i \lambda_i \left( \sum_\sigma \xi_{i\sigma}^+ \xi_{i\sigma} + h_i^+ h_i - 1 \right) - \mu \sum_i h_i^+ h_i,
\]

and a Path-integral formulation of the problem can be written down as usual. In particular, the partition function of the present model is \( 2^N \) times the partition function of the original \( t-J \) model. Notice that the constraint of no double occupancy in our enlarged Hilbert space is imposed by an Lagrange multiplier term as usual.

It is obvious that the same approach can be applied to other models with constraint of no double occupancy, as long as a proper Hamiltonian can be constructed in the enlarged Hilbert space. For example, we find that the Hamiltonian for the Infinite-\( U \) Anderson model in the supersymmetric representation is,

\[
H_{\text{and}} = \sum_{k,\sigma} \epsilon_k a_{k\sigma}^+ a_{k\sigma} + \epsilon_o \sum_{i,\sigma} \xi_{i\sigma}^+ \xi_{i\sigma} + V \sum_{i,\sigma} (a_{i\sigma}^+ \psi_{i\sigma} + \psi_{i\sigma}^+ a_{i\sigma}),
\]

where \( a(a^+)_{k\sigma} \) is the annihilation(creation) operator for conduction electrons with momentum \( \vec{k} \) and spin \( \sigma \) and \( \xi(\xi^+)_{i\sigma} \) are annihilation(creation) operator for localized spins on site \( i \).
where constraint of no double occupancy is imposed. $\epsilon_k$, $\epsilon_o$ and $V$ have their usual meaning in Anderson model. The spin and electron operators in the localized orbitals are represented by $\xi_{i\sigma}$ and $\psi_{i\sigma}$ operators which are supersymmetric in our formulation and the constraint of no double occupancy can be imposed by Langrange multiplier fields as in the $t-J$ model. Notice that the Infinite-$U$ Anderson model is, in fact, completely supersymmetric, in constrast to the $t-J$ model where supersymmetry is broken by $t-$ term.

To see the advantage of present formulation we shall consider in the following the $t-J$ model in the $J = 0$ limit, and shall study the model at two dimension in the mean-field level. The model is equivalent to the $U = \infty$ Hubbard model which is a model of interests in itself [7,8].

A mean-field theory in the supersymmetric $t-(J=0)$-model can be obtained by making the following decouplings,

$$
H \rightarrow -t \sum_{<i,j>,\sigma} \left( <c_{j}\sigma c_{i}\sigma > b_{j}b_{i}^{+} + <b_{j}b_{i}^{+} > c_{j}\sigma c_{i}\sigma > <b_{j}b_{i}^{+} > + c.c. \right)
$$

$$
+ <c_{j}\sigma Z_{i}\sigma > b_{j}f_{i}^{+} + c_{j}\sigma Z_{i}\sigma > <b_{j}f_{i}^{+} > - <c_{j}\sigma Z_{i}\sigma > <b_{j}f_{i}^{+} > + c.c.
$$

$$
+ f_{j}b_{i}^{+} < Z_{j}\sigma c_{i}\sigma > + <f_{j}b_{i}^{+} > Z_{j}\sigma c_{i}\sigma > - <f_{j}b_{i}^{+} > <Z_{j}\sigma c_{i}\sigma > + c.c.
$$

$$
- < Z_{j}\sigma Z_{i}\sigma > f_{j}f_{i}^{+} - Z_{j}\sigma Z_{i}\sigma < f_{j}f_{i}^{+} > + <Z_{j}\sigma Z_{i}\sigma > <f_{j}f_{i}^{+} > + c.c.
$$

$$
+ \lambda \sum_{i,\sigma} (\bar{Z}_{i}\sigma Z_{i}\sigma + c_{i}\sigma ^{+}c_{i}\sigma ) + (\lambda - \mu) \sum_{i} (f_{i}^{+}f_{i} + b_{i}^{+}b_{i})
$$

where $< A >$ is the expectation value of operator $A$ evaluated with the mean-field Hamiltonian. The mean-field parameters $\lambda$ and $\mu$ are chosen so that $< f_{i}^{+}f_{i} + b_{i}^{+}b_{i} > = \delta$ (hole concentration) and $\sum_{\sigma} < \bar{Z}_{i}\sigma Z_{i}\sigma + c_{i}\sigma ^{+}c_{i}\sigma > = 1 - \delta$. We shall be interested at translationally invariant solutions where the mean-field parameters are independent of $<i,j>$ in the following.

Using the fact that $< C > = 0$ for Grassman variables $C$’s, we find that the second and third lines in the mean-field Hamiltonian (11) are equal to zero. However, both slave-boson and slave-fermion type terms are still present in the mean-field Hamiltonian (first and fourth lines in (11)). The relative weight of the two kinds of mean-field terms are determined by the occupation numbers of spins (and holes) with fermion (boson) and boson
(fermion) statistics. These numbers are in term, determined by minimizing the free energy of the system with the constraint that the total number of spins and holes are fixed to be $1 - \delta$ and $\delta$, respectively.

Solving the mean-field equations we find that at low temperatures there are two solutions corresponds to local minima in the mean-field free energy for any given hole concentration $\delta$. The two solutions have either $< c^+c >, < b^+b > \neq 0$ and $< \bar{Z}Z >, < f^+f > = 0$ or the other way around and corresponds to the usual slave-boson and slave-fermion solutions. New solutions where both slave-fermion and slave-boson mean-field parameters are nonzero are also present. However, these solutions correspond to saddle points in free energy landscape and are unstable. Comparing the free energies of the two stable solutions we find that at zero temperature and at low doping $\delta \leq 0.33$ the slave-fermion-like solution has lower energy whereas for $\delta \geq 0.33$ slave-boson-like solution has lower energy. The slave-fermion solution where the spinons condensed with $< Z_{i\uparrow} > = < Z_{i\downarrow} >$ corresponds to ferromagnetic state with spin pointing in $x-$ direction whereas the slave-boson solutions correspond to paramagnetic state. The mean-field theory predicts a first-order transition at zero temperature from ferromagnetic to paramagnetic state as concentration of hole increases across $\sim 0.33$. Notice that numerical [7] and analytical [8] works have established that the Nagaoka (ferromagnetic) state is unstable in the infinite-U Hubbard model for any finite concentration of doping $\delta$ and our mean-field phase diagram is incorrect. Nevertheless, our mean-field theory does produce the qualitative features that the spins (holes) excitations are bosonic (fermionic) like in the ferromagnetic state of the model, and are fermionic (bosonic) like in the paramagnetic state [9].

It has to be emphasized that although the mean-field solutions are either slave-boson or slave-fermion like, spins and holes excitations with both statistics are present in the supersymmetric mean-field theory. For example, in the slave-boson-like solution where $< \bar{Z}Z >, < f^+f > = 0$, bosonic spin and fermionic hole excitations still appear as dispersionless high energy excitations with energies $\lambda$ and $\lambda - \mu$, respectively in the mean-field theory. Similar situation occurs also in the slave-fermion-like solution. The simultaneous appearance
of spin and hole excitations with both statistics in the supersymmetric mean-field theory implies that at finite temperature, the physical properties of the theory is quite different from usual slave-boson or slave-fermion mean-field theories. For example, extra incoherent parts in the one-electron Green’s function which does not exist in usual slave-boson or slave-fermion theories will appear in the supersymmetric theory at nonzero temperature.

At high temperature $T >> \delta(1 - \delta)t$ the only stable mean-field solution which exists is with mean-field parameters $< \bar{Z}Z >, < f^+ f >, < c^+ c >, < b^+ b >$ all equal to zero, indicating that the high-temperature phase is completely incoherent. The transition from coherent low temperature states to incoherent high temperature state is a first-order phase transition in mean-field theory. However, similar results were also obtained in conventional slave-fermion or slave-boson mean-field theories where it is believed that the prediction of first-order phase transition from low-temperature to high-temperature phases is a defect of mean-field theory and should be replaced by a smooth crossover when temperature increases. The mean-field phase diagram is shown in figure 1, where the three stable phases are separated by lines indicating first-order phase transitions in mean-field theory.

Summarizing, by extending the size of Hilbert space, we present in this paper a new way of formulating $t - J$ model where supersymmetry is inherent in the physical observables. The consequence of this hidden supersymmetry is exploited in the $t - J$ model where a new, supersymmetric mean-field theory of the model is introduced and is studied in the $J \rightarrow 0$ limit. The new mean-field theory unifies the slave-boson and slave-fermion mean-field treatments of $t - J$ model by including them as subsets of possible solutions of the new mean-field theory. More generally, new phases where both slave-boson and slave-fermion type mean-field parameters are nonzero may also exist.

Perhaps the more important message in this paper is the demonstration of existence of supersymmetry in general strongly correlated systems where the low energy physics is described by effective Hamiltonians with constraint of no double occupancy like the $t - J$ or infinite-$U$ Anderson model. The consequence of this supersymmetry is never exploited in studies of strongly-correlated systems. Note that supersymmetry is broken by the $t-$ term.
in the $t - J$ model and it’s consequences are not fully exploited in our paper presenting only the mean-field treatment of $t - (J = 0)$ model. Further studies of the $t - J$ model is underway and the results will be presented in future papers.

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REFERENCES

[1] P.W. Anderson, Science 235, 1196 (1987).

[2] G. Baskaran, Z.Zou and P.W. Anderson, Solid State Commun. 63, 973 (1987); C. Gros, R. Joynt and T.M. Rice, Phys. Rev. B 36, 8190 (1987); G. Kotliar and J. Liu, Phys. Rev. B 38, 5142 (1988).

[3] C. Jayaprakash, H.R. Krishnamurthy, and S. Sarker, Phys. Rev. B 40, 2610 (1989); C.L. Kane, P.A. Lee, T.K. Ng, B. Chakraborty and N. Read, Phys. Rev. B 41, 2653 (1990).

[4] X.-G. Wen and P.A. Lee, Phys. Rev. Lett. 76, 503 (1996).

[5] P.A. Lee, N. Nagaosa, T.K. Ng and X.-G. Wen, to appear in Phys. Rev. B

[6] S.C. Zhang, Science 275, 1089 (1997).

[7] W.O. Putikka, M.U. Luchini and M. Ogata, Phys. Rev. Lett. 69, 2288 (1992).

[8] B.S. Shastry, H.R. Krishnamurthy and P.W. Anderson, Phys. Rev. B 41, 2375 (1990); S.-Q. Shen, Z.-M. Qiu and G.-S. Tian, Phys. Lett. A178, 426 (1993).

[9] W. Long and X. Zotos, Phys. Rev. B 48, 317 (1993).
FIGURES

FIG. 1. phase diagram of the $t(J = 0)$ model in supersymmetric mean-field theory: (HT)-high temperature phase, (SB)-slave-boson-like phase, (SF)-slave-fermion-like phase
Phase Diagram

HT

SF

SB

T/t

delta