Formation of energy gap in higher dimensional spin-orbital liquids

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A Schwinger boson mean field theory is developed for spin liquids in a symmetric spin-orbital model in higher dimensions. Spin, orbital and coupled spin-orbital operators are treated equally. We evaluate the dynamic correlation functions and collective excitations spectra. As the collective excitations have a finite energy gap, we conclude that the ground state is a spin-orbital liquid with a two-fold degeneracy, which breaks the discrete spin-orbital symmetry. Possible relevance of this spin liquid state to several realistic systems, such as CaV\(_4\)V\(_9\) and Na\(_2\)Sb\(_2\)Ti\(_3\)O, are discussed.

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The formation of a spin gap in two- or higher dimensional quantum spin systems is a long-standing issue in strongly correlated problems. Several physical mechanisms were proposed to explain the formation of the spin gap in the low-energy excitations. Most of them focus on one-dimensional spin chains and spin ladders, such as an S=1 antiferromagnetic Heisenberg chain and even-leg spin ladders. In higher dimensions Anderson proposed that strong quantum fluctuations for spin-1/2 systems may destroy the antiferromagnetic long-range order in two dimension, and lead to form a resonating valence bond (RVB) state where a spin gap may open. However, it becomes true only for some frustrated spin systems such as on the Kagome lattice or in the Majumdar-Ghosh model with a strong next nearest neighbor interaction, otherwise there exists antiferromagnetic long-range orders in the ground state on a square and triangle lattice. Recently it has been realized that orbital degrees of freedom of d- and f-electrons in transition metal ions provide a new route to find the physical mechanism of spin gap formation. Several spin-orbital models have shown the tendency of the formation of a spin gap in the ground states due to strong orbital and spin quantum fluctuations. Accumulating numerical calculations show that spin liquid state may be formed in some one-dimensional spin-orbital coupled systems. Behaviors in higher dimensional systems are relatively less clear. There are several higher dimensional spin-gap materials such as Na\(_2\)Ti\(_2\)Sb\(_2\)O\(_4\) and NaV\(_4\)O\(_9\), in which the orbital degree of freedom might play a key role in the formation of the spin gap.

The spin-orbital model Hamiltonian is written as

\[
H = J \sum_{\langle ij \rangle} \left( 2 \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \right) \left( 2 \mathbf{\tau}_i \cdot \mathbf{\tau}_j + \frac{1}{2} \right) + J_s \sum_{\langle ij \rangle} \left( 2 \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \right) + J_r \sum_{\langle ij \rangle} \left( 2 \mathbf{\tau}_i \cdot \mathbf{\tau}_j + \frac{1}{2} \right). \tag{1}
\]

This model may be derived from an electronic model with double orbital degeneracy. This model possesses an SU(2) \(\otimes\) SU(2) symmetry. When \(J_s = J_r = J_0\), the model have an additional discrete symmetry, namely, the permutation symmetry between spin and orbital. In this case the model can be written as a combination of two symmetric models

\[
H = (J + J_0) \sum_{\langle ij \rangle} \left( 2 \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \right) \left( 2 \mathbf{\tau}_i \cdot \mathbf{\tau}_j + \frac{1}{2} \right) - J_0 \sum_{\langle ij \rangle} \left( 2 \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{2} \right) \left( 2 \mathbf{\tau}_i \cdot \mathbf{\tau}_j - \frac{1}{2} \right). \tag{2}
\]

The former part is the standard SU(4) spin-orbital model, which is solvable in one-dimension and has been investigated intensively. The second part is the model first proposed by Santoro, and also possesses the SU(4) symmetry with different generators. However the combination of the two models breaks the SU(4) symmetry.

From previous studies, it has been found that the interplay between spin and orbital degrees of freedom produces either quantum ordered or disordered phases. Spin liquid states with an energy gap were found in one dimensions. To investigate the model systematically, we try to develop a simple theory, which can describe the disordered state with an energy gap as well as the ordered states. The Schwinger boson theory is an ideal candidate. The theory was first used to the spin SU(2) Heisenberg model, and then was generalized to SU(N) systems. The advantage of this theory is that it can describe either quantum ordered or disordered states. The results for two- and three-dimensional Heisenberg model are consistent with the spin wave theory very well. Here we present the Schwinger boson mean field theory for this spin-orbital system.

For the present model, there are four possible states on each site \(i\) according to the eigenvalues of \(\mathbf{S}_i^z\) and \(\mathbf{\tau}_i^z\): \(|1\rangle = |+1/2, +1/2\rangle, |2\rangle = |-1/2, +1/2\rangle, |3\rangle = |+1/2, -1/2\rangle, |4\rangle = |-1/2, -1/2\rangle\). We introduce four Schwinger bosons to describe these four states: \(\mu = a_{\mu}^\dagger |0\rangle\), where \(|0\rangle\) is the vacuum states and \(\mu = 1, 2, 3, 4\). There is a constraint for the four bosons: \(\sum_{\mu=1}^{4} a_{\mu}^\dagger a_{\mu} = 1\), for each site. On these basis the spin and orbital operators can be expressed in terms of these four Schwinger

\[
|1\rangle = |+1/2, +1/2\rangle, |2\rangle = |-1/2, +1/2\rangle, |3\rangle = |+1/2, -1/2\rangle, |4\rangle = |-1/2, -1/2\rangle. \tag{3}
\]

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\]
bosons.

\[ S_i^+ = a_i^\dagger a_{i2} + a_i^\dagger a_{i4}; \quad \tau_i^+ = a_i^\dagger a_{i3} + a_i^\dagger a_{i4}; \]

\[ S_i^- = a_i^\dagger a_{i1} + a_i^\dagger a_{i3}; \quad \tau_i^- = a_i^\dagger a_{i1} + a_i^\dagger a_{i2}; \]

\[ S_i^z = \frac{1}{2} (a_i^\dagger a_i - a_i a_i) = \frac{1}{2} (a_i^\dagger a_i - a_i a_i); \quad \tau_i^z = \frac{1}{2} (a_i^\dagger a_i - a_i a_i); \]

Thus, the Hamiltonian is rewritten in terms of the Schwinger bosons

\[ H = \frac{-\langle J + J_0 \rangle}{2} \sum_{(ij), \mu \nu} A_{ij, \mu \nu}^\dagger A_{ij, \mu \nu} \]

\[ -J_0 \sum_{(ij), \mu \nu} (B_{ij,14}^\dagger - B_{ij,23}^\dagger)(B_{ij,14} - B_{ij,23}) \]

\[ + \sum_i \lambda_i (\sum_{\mu} a_i^\dagger a_i - 1) + \frac{1}{2} z N_A (J + 2J_0) \tag{3} \]

where \( A_{ij, \mu \nu} = a_{i\mu} a_{j\nu} - a_{i\nu} a_{j\mu} \) and \( B_{ij, \mu \nu} = a_{i\mu} a_{j\nu} + a_{i\nu} a_{j\mu} \). We have introduced antisymmetric and symmetric operators \( A \) and \( B \) for the purpose of the mean field calculations. The following theory is limited to the case \( -J \geq J_0 \geq 0 \). We should introduce different order parameters in the different parameter range. The local Lagrangian multiiplier is introduced to realize the local constraint for hard core bosons. In the mean field approach we shall take it as site-independent \( \lambda \). The thermodynamic averages of the operators \( A \) and \( B \) are introduced as the order parameters, respectively,

\[ \langle A_{ij, \mu \nu} \rangle = -2i \Delta_{ij, \mu \nu}^o (r_i - r_j); \quad \langle B_{ij, \mu \nu} \rangle = 2 \Delta_{ij, \mu \nu}^e (r_i - r_j). \]

\( \Delta_{ij, \mu \nu}^o (r_i - r_j) \) and \( \Delta_{ij, \mu \nu}^e (r_i - r_j) \) are odd and even functions with respect to the indices \( \mu, \nu \) or the sites \( r_i, r_j \). In the momentum space, we take

\[ \frac{i}{Z} \sum_{\delta} \Delta_{ij, \mu \nu}^o (\delta) e^{-ik \cdot \delta} \equiv \Delta_{ij, \mu \nu}^o \gamma_o (k); \]

\[ \frac{1}{Z} \sum_{\delta} \Delta_{ij, \mu \nu}^e (\delta) e^{-ik \cdot \delta} \equiv \Delta_{ij, \mu \nu}^e \gamma_e (k); \]

where \( \Delta \) points to the nearest neighbor sites. By utilizing the Pauli matrices \( \sigma_\alpha (\alpha = x, y, z) \) and the identity matrix \( \sigma_0 \), the decoupled Hamiltonian can be expressed in a compact form of \( 8 \times 8 \) matrix,

\[ H = \frac{1}{2} \sum_k \Phi_k^\dagger H(k) \Phi_k + \mathcal{E}_0 \]

where

\[ \Phi_k = (a_{k1}^\dagger, a_{k2}^\dagger, a_{k3}^\dagger, a_{k4}^\dagger, a_{-k1}, a_{-k2}, a_{-k3}, a_{-k4}); \]

\[ H(k) = \lambda \sigma_0 \otimes \sigma_0 \otimes \sigma_0 - i \sigma_y \otimes A(k) + b(k) \sigma_x \otimes \sigma_y \otimes \sigma_y; \]

\[ A(k) = -2z(J + J_0) \gamma_o \cdot k \begin{pmatrix} 0 & \gamma_{12} & \gamma_{13} & \gamma_{14} \\ -\gamma_{12} & 0 & \gamma_{23} & \gamma_{24} \\ -\gamma_{13} & -\gamma_{23} & 0 & \gamma_{24} \\ -\gamma_{14} & -\gamma_{24} & -\gamma_{24} & 0 \end{pmatrix}; \]

\[ \mathcal{E}_0 = z(J + J_0) \sum \Delta_{ij, \mu \nu}^2 + 2zJ_0 (\Delta_{ij, \mu \nu}^2)^2 - 3\lambda + \frac{1}{2} z (J + 2J_0), \]

where \( b(k) = -2z(J + J_0) \Delta_{ij, \mu \nu}^o \gamma_o (k) \). The Kronecker product for block matrices is used. [14] The Hamiltonian can thus be diagonalized analytically, and the free energy is evaluated to establish the mean field equations. Due to the symmetry in the Hamiltonian, there exist two sets of solutions: (I) \( \Delta_{ij, \mu \nu}^o = \Delta_{ij, \mu \nu}^e = \Delta \) with \( \Delta = \sqrt{\Delta_{ij, \mu \nu}^o + \Delta_{ij, \mu \nu}^e}; \) (II) \( \Delta_{ij, \mu \nu}^o = \Delta_{ij, \mu \nu}^o = -\Delta_{ij, \mu \nu}^e = -\Delta_{ij, \mu \nu}^e \) and \( \Delta_{ij, \mu \nu}^o = \Delta_{ij, \mu \nu}^e = \Delta_{ij, \mu \nu}^e = \Delta_{ij, \mu \nu}^e \). With the notation \( \Delta, \Delta_1, \Delta_2 \), and the same branches of spectra are given by

\[ \omega(k) = \sqrt{k^2 - [2z(J + J_0) \gamma_o]_2 (\Delta_{ij, \mu \nu}^o + \Delta_{ij, \mu \nu}^e)}, \tag{4} \]

where \( a(k) = -2z(J + J_0) \Delta_{ij, \mu \nu}^o \gamma_o (k) \) and \( b(k) = -2z(J + J_0) \Delta_{ij, \mu \nu}^o \gamma_o (k) \). Moreover, these two ground states are degenerated. The degeneracy originates from the symmetry of permutation of spin and orbital operators. When \( J_0 = 0 \), the model is reduced to the standard SU(4) spin-orbital model. The two spectra become degenerated,

\[ \omega(k) = \sqrt{\lambda^2 - [2z(J + J_0) \gamma_o (k)]^2 (\Delta_{ij, \mu \nu}^o + \Delta_{ij, \mu \nu}^e)}, \]

This way we recover the spectra for the SU(N=4) model.

In the following we will focus on the ground state with an energy gap. So we do not consider the Bose-Einstein condensation which may give rise to the long-range order. Indeed the long-range orders appear when \( J_0 = 0 \) or \( J = J_0 \) on two- and three-dimensional hypercubic lattices. [15] The condensation occurs when the system deviates from those symmetric point slightly. General description of complete solutions to the problem will be presented elsewhere. To determine the order parameters, we introduce a set of dimensionless parameters \( \Delta = 2z(J + J_0) \Delta / \lambda, \Delta_1 = 2z(J + J_0) \Delta_1 / \lambda, \Delta_2 = 2zJ_0 \Delta_2 / \lambda, \) and \( \lambda = \lambda / [z(J + J_0)] \), then the quasiparticle excitation spectrum becomes

\[ \tilde{\omega}_k^o (k) = \sqrt{1 - \Delta^2 (J + J_0)} - \Delta_1 \gamma_o (k) \pm \Delta_2 \gamma_e (k), \tag{5} \]

The self-consistent mean field equations are given by

\[ \int \frac{dk}{(2\pi)^d} \left[ \frac{1}{\tilde{\omega}_+ (k)} + \frac{1}{\tilde{\omega}_- (k)} \right] = 3 \tag{6} \]

\[ \int \frac{dk}{(2\pi)^d} \left[ \gamma_o^2 (k) + \gamma_e^2 (k) \right] = 2 \lambda \tag{7} \]
\[
\int \frac{dk}{(2\pi)^d} \left[ \frac{(\Delta_1 \gamma_0(k) + \Delta_2 \gamma_0(k)) \gamma_0(k)}{\omega_+(k)} + \frac{(\Delta_1 \gamma_0(k) - \Delta_2 \gamma_0(k)) \gamma_0(k)}{\omega_-(k)} \right] = 2\tilde{\Delta}_1 \tag{8}
\]
\[
\int \frac{dk}{(2\pi)^d} \left[ \frac{(\Delta_1 \gamma_0(k) + \Delta_2 \gamma_0(k)) \gamma_0(k)}{\omega_+(k)} - \frac{(\Delta_1 \gamma_0(k) - \Delta_2 \gamma_0(k)) \gamma_0(k)}{\omega_-(k)} \right] = \tilde{\lambda} \Delta_2 (1 + \frac{J}{J_0}). \tag{9}
\]
Substituting Eq. (8) into Eq. (9), we have
\[
\int \frac{dk}{(2\pi)^d} \left[ \frac{1}{\omega_+(k)} - \frac{1}{\omega_-(k)} \right] \tilde{\Delta}_2 \gamma_0(k) \gamma_0(k) = 0.
\]
If \( \tilde{\Delta}_2 \neq 0 \), \( \tilde{\Delta}_1 \) must be equal to zero. Oppositely, if \( \tilde{\Delta}_2 = 0 \), the solution is for the case of \( J_0 = 0 \). Therefore for \( J_0 > 0 \), the solution is \( \tilde{\Delta}_1 = 0 \) with \( \omega_+(k) = \omega_-(k) \). The two spectra are also degenerated. Two sets of saddle point solutions become, corresponding to the spin liquid phase with an energy gap in elementary excitations: (I) \( \Delta_{14} = \Delta_{23} = 0 \), \( \Delta_{12} = 0 \), \( \Delta = 0 \), and \( \Delta_{10} = 0 \) otherwise. (II) \( \Delta_{14} = \Delta_{23} = 0 \), \( \Delta_{12} = -\Delta_{24} = 0 \), \( \Delta = 0 \), \( \Delta_{10} = 0 \) otherwise. We focus on the first set of solutions and then present the results for the second set of solutions.

The one-particle Green’s function in an \( 8 \times 8 \) matrix form is defined as
\[
G(k, t) = -i \left\langle 0 | T \{ \Phi_k(t) \Phi_k^\dagger(0) \} | 0 \right\rangle
\]
where \( | 0 \rangle \) is the ground state of the Hamiltonian. Its Fourier transform is given by
\[
G(k, \omega) = ((\omega + i\delta) \sigma_z \otimes \sigma_0 \otimes \sigma_0 - H_k)^{-1}
\]
\[
= \frac{1}{\omega^2 - \lambda^2 + a^2(k) + b^2(k) + i\delta} \times
\left\{ \omega \sigma_z \otimes \sigma_0 \otimes \sigma_0 - \lambda \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + a(k) \sigma_y \otimes \sigma_0 \otimes \sigma_y - b(k) \sigma_x \otimes \sigma_y \otimes \sigma_y \right\},
\]
with \( a(k) = -2z(J + J_0) \Delta \gamma_0(k) \) and \( b(k) = -2z J_0 \Delta \gamma_0(k) \). The corresponding saddle point equations then become:
\[
\int \frac{dk}{(2\pi)^d} \frac{1}{\omega_+(k)} = \frac{3}{2};
\]
\[
\int \frac{dk}{(2\pi)^d} \frac{\gamma_0^2(k)}{\omega(k)} = \tilde{\lambda};
\]
\[
\int \frac{dk}{(2\pi)^d} \frac{\gamma_0^2(k)}{\omega(k)} = \frac{1}{2} \tilde{\lambda} (1 + \frac{J}{J_0}).
\]
For a given value of \( J/J_0 \), we have a set of solutions for \( \tilde{\lambda}, \tilde{\Delta} \). Our solutions in this paper are limited to \( \min(\omega(k)) \neq 0 \). To determine the physical properties, we evaluate the dynamic correlation functions for the spin \( S_z^2 \), orbital \( T_z^2 \), and spin-orbital density operators \( 2S_z^2 T_z^2 \). After some algebra, we have
\[
\chi_x(q, \Omega + i\delta) = \frac{1}{8} \int \frac{dk}{(2\pi)^d} \left[ \frac{C_X(k, q)}{\omega(k) \omega(k + q)} - 1 \right]
\]
\[
= \frac{1}{\Omega + i\delta + \omega(k) + \omega(k + q) - \Omega + i\delta - \omega(k) - \omega(k + q)}
\]
with \( (X = S, T, ST) \)
\[
C_S(k, q) = \lambda^2 - a(k) a(k + q) - b(k) b(k + q);
\]
\[
C_T(k, q) = \lambda^2 + a(k) a(k + q) - b(k) b(k + q);
\]
\[
C_{ST}(k, q) = \lambda^2 - a(k) a(k + q) + b(k) b(k + q).
\]
There are a set of relations
\[
\chi_S(0, \Omega) = 0;
\]
\[
\chi_T(0, \Omega) = \chi_{ST}(Q, \Omega);
\]
\[
\chi_T(Q, \Omega) = \chi_{ST}(0, \Omega);
\]
\[
\chi_S(Q, \Omega) = \chi_T(0, \Omega) + \chi_{ST}(Q, \Omega) = \chi_{ST}(0, \Omega) + \chi_{ST}(Q, \Omega),
\]
where for \( \Omega > 0 \)
\[
\text{Im}[\chi_T(0, \Omega)] = \frac{\pi}{4} \int \frac{dk}{(2\pi)^d} \frac{a^2(k)}{\omega^2(k)} \delta(\Omega - 2\omega(k));
\]
\[
\text{Im}[\chi_T(Q, \Omega)] = \frac{\pi}{4} \int \frac{dk}{(2\pi)^d} \frac{b^2(k)}{\omega^2(k)} \delta(\Omega - 2\omega(k)).
\]
If the minimum of \( \omega(k) \) is non-zero, \( \text{Im}[\chi_x(q, \Omega)] \) become non-zero ONLY when \( \Omega \geq 2 \min(\omega(k)) \). Thus the collective excitations for the density-density correlation function have a finite energy gap, \( \Delta_{gap} = 2 \min(\omega(k)) \). It is worth mentioning that the solution has broken the discrete permutation symmetry of spin and orbital. This can be seen from the fact that, in general, \( \chi_S(q, \Omega) \neq \chi_T(q, \Omega) \). The same expressions are obtained for the second set of solutions if we permute the indices \( S \) and \( T \). The spectra and free energy as well as the energy gap are identical to the first set of solutions. Thus the two sets of solutions are energetically degenerated. The symmetries in the two states are different. More important, the double degeneracy of the ground state was also observed in one-dimensions in other approaches. [13]

Therefore, this two-fold degeneracy is not a consequence of the mean field approaches and can be regarded as an evidence to support our mean field theory.

Now we come to evaluate the energy gap by solving the mean field equations. On a one-dimensional chain, the energy gap can be evaluated analytically by introducing a parameter \( x_0 = (\Delta^2 - \Delta^2_0)/(1 - \Delta^2) \). The energy gap and the ratio of \( J_0/J \) are
\[
\Delta_{gap} = 4z(J + J_0) \times \left\{ \frac{K(x_0) - E(x_0)}{1 - x_0 K(x_0) - E(x_0)} \right\}, \quad \text{if } x_0 < 0;
\]
\[
\frac{J}{J_0} = -1 + 2 \frac{K(x_0) - E(x_0)}{E(x_0) - (1 - x_0) K(x_0)}, \quad \text{if } x_0 \geq 0;
\]
where \( K(x) \) is the complete elliptic integral of the second kind and \( E(x) \) is the complete elliptic integral of the first kind. We have established a one-to-one correspondence between the ratio \( J_0/J \) and the energy gap. We find that there is a turning point at \( J_0/J = 1 \). The theory fails at the symmetric point \( J_0 = 0 \). The energy gap still opens
at that point, which is in conflict with the solution of Bethe ansatz. The same problem was encountered in the spin-1/2 SU(2) theory in one dimension.

![Diagram](image)

**FIG. 1.** The energy gap via the ratio of $J_0/J$ in two- and three-dimensions.

The energy gaps for two- and three-dimensional lattices are plotted in Fig.1. We find that the energy gap opens in the regime of $0.380 < J_0/J < 9.84$ for $d = 2$ and of $0.666 < J_0/J < 1.667$ for $d = 3$. The gap closes at two critical ratios $J_0/J$. From Fig.1, it is shown that the energy gap appears in a larger parameter range in two-dimension than in three dimension. This is consistent with the fact that the quantum fluctuations are stronger in two dimension. Out of the above parameter regimes the Bose condensations have to be considered, otherwise the mean field equations have no solutions. In this case the ground state may possess long-range orders as we discussed in the symmetric point $J = -J_0$. We shall discuss these phases elsewhere. As far as we know the Schwinger boson mean field theory is very successful for the spin liquid state for $s = 1$ in one dimension, and antiferromagnetic states for higher dimensions. Our theory shows it also works very well for spin-orbital liquid states in higher dimensions.

The formation of a spin energy gap indicates that the ground state is a spin-orbital liquid. Experimentally the energy gap can be measured from magnetic susceptibility. There are several higher-dimensional materials such as Na$_2$Ti$_2$Sb$_2$O and CaV$_4$O$_9$. It is believed that the orbital degrees of freedom plays an important role in the formation of spin gap. The low temperature phases of these materials may be relevant to the spin-orbital liquid with the energy gap as we discuss in this paper.

In conclusion we develop a Schwinger boson mean field theory for the formation of a spin-gap in any dimensions. The ground state of the model is a spin-orbital liquid with an energy gap in an extensive parameter regime. This ground state breaks the discrete symmetry of permutation of spin and orbital, and is doubly degenerated.

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