Spin and quadrupole correlations in the insulating nematic phase of spin-1 bosons in optical lattices

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We consider the effective model of $H = -J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J_2 \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2$, describing the Mott insulating state with odd number of spin-1 bosons in optical lattices ($J_2 > J_1 > 0$). In terms of an SU(3) boson representation, a valence bond mean field theory is developed. In 1D, a first-order quantum phase transition from a spin singlet to a spin nematic phase with gapful excitations is identified at $J_1/J_2 = 0.19833$, while on a 2D square lattice a spin nematic ordered phase with gapless excitations prevails. In both 1D and 2D cases, we predict that the spin structure factor displays dominant antiferromagnetic fluctuations, while the quadrupole structure factor exhibits strong ferroquadrupolar correlations.

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Degenerate alkali atoms are considered weakly interacting boson gas due to the smallness of the scattering length compared with the inter-particle separation. However, the situation changes dramatically when an optical potential created by standing laser beams confines particles in valleys of the periodic potential and strongly enhances local interactions. Recently, the nontrivial Mott insulating state of bosonic atoms in optical lattices has been demonstrated experimentally [1]. In addition to solid state systems, spinor atoms in optical lattices provide a novel realization of quantum magnetic systems with the possibility to tune various parameters of the effective models in the absence of disorder [2, 3, 4].

Alkali atoms have a nuclear spin $3/2$. Lower energy hyperfine manifold has three magnetic sublevels and a total moment $S = 1$. In order to observe the quantum spin phenomena experimentally, one has to consider a system with small number of particles and strong interactions. In the insulating state, atoms are localized, and fluctuations in the particle number on each site are suppressed. Virtual tunnelling of atoms between neighboring sites induces effective spin interactions, leading to novel quantum magnetic phases [2, 3, 4, 5].

The boson-Hubbard model is used to describe the low-energy physics of spin-1 bosonic atoms in an optical lattice [5].

$$H = -t \sum_{\langle i,j \rangle,m} (a_{i,m}^\dagger a_{j,m} + h.c.) + \frac{U_0}{2} \sum_{i} n_i (n_i - 1)$$
$$+ \frac{U_2}{2} \sum_{i} (S_i^2 - 2n_i) - \mu \sum_{i} n_i,$$

(1)

where $n_i = \sum_{m} a_{i,m}^\dagger a_{i,m}$ and $S_i^\alpha = \sum_{m,n} a_{i,m}^\dagger T_{m,n}^\alpha a_{i,n}$ denote the number of atoms and the spin operator on the $i$ site ($m = -1, 0, 1$), respectively, while $T_{m,n}^\alpha$ denote the matrices for the spin-1 particles.

In the $t = 0$ limit with odd number of bosons per site, the bosonic symmetry of the wave function requires that each site has a localized spin with odd quantum numbers. The interactions of Eq.(1) are minimized when the localized spins take the smallest possible value $S = 1$. Away from this limit, the second order perturbation theory in $t$ leads to an effective spin superexchange model [6, 7, 10].

$$H = -J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J_2 \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2,$$

(2)

where the coupling parameters are confined to $0 < J_1/J_2 < 1$. For a two-spin problem, the first term favors a polarized configuration, while the second prefers a spin singlet form. Thus, the effective model acts as a spin-1 Heisenberg antiferromagnet with ferromagnetic frustrations.

It has been an outstanding issue to study the ground states of this effective model [6, 7, 10, 11, 12]. More exotic ground states may be realized in 1D [8, 13, 14], but there is no consensus yet. In this paper, using an SU(3) boson representation, we develop a valence bond mean field (MF) theory. In 1D, a first-order quantum phase transition is found from a spin singlet ($J_1/J_2 < 0.19833$) to a (short-range ordered) spin nematic phase ($J_1/J_2 > 0.19833$) with gapful excitations, while on a 2D square lattice an ordered spin nematic phase is always obtained. Moreover, the spin and quadrupole correlation spectra in both disordered and ordered nematic phases are calculated explicitly, to be checked by future experiments.

To describe the spin-1 operators, an SU(3) bosonic representation is defined by generators $F_{m}^{\alpha}(i) = a_{i,m}^\dagger a_{i,n}$, where indices $m$ and $n$ specify the spin projection with values $-1, 0, 1$. The commutation relation is satisfied

$$[F_{m}^{n}(i), F_{\mu}^{\nu}(j)] = \delta_{i,j} \left[ \delta_{\mu,\nu} F_{m}^{\nu}(i) - \delta_{m,\nu} F_{m}^{\mu}(i) \right],$$

(3)

which forms an SU(3) Lie algebra. The corresponding spin operators are expressed as $S_i^+ = \sqrt{2} (a_{i,0}^\dagger a_{i,-1} + a_{i,-1}^\dagger a_{i,0})$, $S_i^- = (S_i^+)^\dagger$, $S_i^z = (a_{i,1}^\dagger a_{i,1} - a_{i,-1}^\dagger a_{i,-1})$. With
this boson representation, we can verify $[S_i^+, S_j^-] = 2S_i^x \delta_{ij}$, $[S_i^z, S_j^\pm] = \pm S_i^\pm \delta_{ij}$. In order to fix $S_i^z = S(S+1) = 2$, a local constraint $\sum_m a_i^\dagger a_i m = 1$ has to be imposed.

To make the spin representation symmetric, linear combinations are introduced: $b_{i,1} = \frac{1}{\sqrt{2}}(a_i -1 - a_i)$, $b_{i,2} = \frac{1}{\sqrt{2}}(a_i -1 + a_i)$, and $b_{i,3} = a_i \delta_{i,0}$, and the spin (dipolar) operators are written in antisymmetric form

$$
\begin{align*}
S_i^{xy} &= -i(b_{i,2} b_{i,3} - b_{i,3} b_{i,2}), \\
S_i^{xy} &= -i(b_{i,3} b_{i,1} - b_{i,1} b_{i,3}), \\
S_i^{xy} &= -i(b_{i,1} b_{i,2} - b_{i,2} b_{i,1}).
\end{align*}
$$

and the local constraint holds as $\sum_\alpha b_{i,\alpha} b_{i,\alpha} = 1$. Actually for spin-1 bosonic atoms, quadrupole operators can be defined by

$$
Q_i^{(0)} = 3(S_i^x)^2 - 2 = b_{i,1} b_{i,1} + b_{i,2} b_{i,2} - 2b_{i,3} b_{i,3}, \\
Q_i^{(2)} = (S_i^y)^2 - (S_i^y)^2 = -(b_{i,1} b_{i,1} b_{i,2} b_{i,2}), \\
Q_i^{xy} = S_i^x S_i^y + S_i^y S_i^x = -(b_{i,3} b_{i,2} + b_{i,2} b_{i,3}), \\
Q_i^{xz} = S_i^x S_i^z + S_i^z S_i^x = -(b_{i,3} b_{i,1} + b_{i,1} b_{i,3}), \\
Q_i^{yz} = S_i^y S_i^z + S_i^z S_i^y = -(b_{i,2} b_{i,3} + b_{i,3} b_{i,2}).
$$

Three dipole and five quadrupole operators form generators of the SU(3) Lie group, as in the Gell-Mann matrix representation. Then, the effective spin model is expressed as:

$$
H = -\sum_{i<j>\alpha,\beta} \left[ J_1 b_{i,\alpha}^\dagger b_{i,\beta} b_{j,\beta}^\dagger b_{j,\alpha} \right] + (J_2 - J_1) b_{i,\alpha}^\dagger b_{i,\beta} b_{j,\beta}^\dagger b_{j,\alpha}.
$$

In the limit $J_1 = J_2$, the model is reduced to an SU(3) symmetric ferromagnetic superexchange model, invariant under the uniform SU(3) transformation, for which the spin ferromagnetic and spin nematic long-range order can coexist in higher dimensions [13]. On the other hand, in the limit $J_1 = 0$, the model is reduced to an SU(3) symmetric valence-bond antiferromagnetic model, invariant under the staggered conjugate transformations of the two sublattices, leading to a spin dimerization in 1D [14, 15].

It is shown that an SU(2) Schwinger boson MF theory can describe rather well the spin correlations for spin-1/2 Heisenberg antiferromagnets [16]. To develop a similar valence bond MF theory, we introduce symmetric pairing parameters

$$
\begin{align*}
\Delta_{1,1} &= -\langle b_{i,1}^\dagger b_{j,1}^\dagger \rangle, \\
\Delta_{1,2} &= -\langle b_{i,1}^\dagger b_{j,2}^\dagger + b_{i,2}^\dagger b_{j,1}^\dagger \rangle, \\
\Delta_{1,3} &= -\langle b_{i,1}^\dagger b_{j,3}^\dagger + b_{i,3}^\dagger b_{j,1}^\dagger \rangle, \\
\Delta_{2,3} &= -\langle b_{i,2}^\dagger b_{j,3}^\dagger + b_{i,3}^\dagger b_{j,2}^\dagger \rangle.
\end{align*}
$$

To preserve the SU(2) spin rotational symmetry of the model, we have to assume $\Delta_{1,1} = \Delta_{2,2} = \Delta_{3,3} \equiv \Delta_0$ and $\Delta_{1,2} = \Delta_{3,1} = \Delta_{2,3} \equiv \Delta_0$. By introducing a Nambu spinor $\Psi_k = (b_{k,1}^\dagger, b_{k,2}^\dagger, b_{k,3}^\dagger, b_{-k,1}, b_{-k,2}, b_{-k,3})$, we can rewrite the MF Hamiltonian in a matrix form

$$
H_{mf}(k) = \frac{1}{2} \sum_k \Psi_k^\dagger H_{mf}(k) \Psi_k \\
+ \frac{3}{2} \left( (3J_2 - J_1) \Delta_0^2 + J_1 \Delta_0^2 \right) Nz - \frac{5}{2} \lambda N,
$$

where the local constraint has been implemented by a Lagrangian multiplier $\lambda$, $N$ the total number of lattice sites, and $z$ the number of the nearest neighbor sites. The MF Hamiltonian matrix is given by

$$
H_{mf}(k) = \lambda + 2\Delta_0(k) \sigma_z \otimes I + \Delta_0(k) \sigma_x \otimes M,
$$

where $M$ is the $3 \times 3$ unit matrix, $\sigma_\alpha$ ($\alpha = x, y, z$) are Pauli matrices, $\Delta_\alpha(k) = \frac{\gamma}{\Delta_0} (3J_2 - J_1) k$ and $\gamma = \frac{1}{2} \sum_\delta \cos k \cdot \delta$ and $\delta$ the nearest neighbor vector. The corresponding Matsubara Green function (GF) is thus deduced to

$$
G^{-1}(k, i\omega_n) = i\omega_n \sigma_z \otimes I - H_{mf}(k),
$$

where $\omega_n$ is the bosonic Matsubara frequency. The poles of the GF matrix give rise to the quasiparticle spectra: $\epsilon_1(k) = \sqrt{\lambda^2 - 4(\Delta_0(k) + \Delta_b(k))^2}$ and $\epsilon_2(k) = \sqrt{\lambda^2 - (2\Delta_0(k) - \Delta_b(k))^2}$, where the lower band $\epsilon_1(k)$ is singly occupied while the higher band $\epsilon_2(k)$ is doubly degenerate.

From the free energy of the system, the saddle point equations at $T = 0K$ are derived as

$$
\begin{align*}
\frac{1}{N} \sum_k \left[ \frac{\lambda}{2\epsilon_1(k)} + \frac{\lambda}{\epsilon_2(k)} \right] &= \frac{5}{2}, \\
\frac{1}{N} \sum_k \frac{\gamma^2}{\epsilon_1(k)} &= \frac{2(\Delta_0 + \Delta_b)}{z ((3J_2 - J_1) \Delta_0 + 2J_1 \Delta_b)}, \\
\frac{1}{N} \sum_k \frac{\gamma^2}{\epsilon_2(k)} &= \frac{2\Delta_0 - \Delta_b}{z ((3J_2 - J_1) \Delta_0 - J_1 \Delta_b)}.
\end{align*}
$$

while the ground state energy is $E_g = -\frac{\gamma}{2} z N \left[ (3J_2 - J_1) \Delta_0^2 + J_1 \Delta_b^2 \right]$. From the GF matrix, we can also derive the double-time GFs of the boson operators

$$
\langle \langle b_{k,2} b_{k,1}^\dagger \rangle \rangle = \langle \langle b_{k,3} b_{k,2}^\dagger \rangle \rangle = \langle \langle b_{k,3} b_{k,3}^\dagger \rangle \rangle = \frac{\lambda}{2\epsilon_1(k)} + \frac{\lambda}{\epsilon_2(k)} \\
= \frac{\lambda}{2\epsilon_1(k)} + \frac{\lambda}{\epsilon_2(k)},
$$

and $\langle \langle b_{k,1} b_{k,1}^\dagger \rangle \rangle = \langle \langle b_{k,2} b_{k,2}^\dagger \rangle \rangle = \langle \langle b_{k,3} b_{k,3}^\dagger \rangle \rangle$. Using the spectral representation, we can calculate the expectation
values at \( T = 0 \)K,
\[
\langle b_{i_1}^\dagger b_{i_2} \rangle = \langle b_{i_2}^\dagger b_{i_3} \rangle = \langle b_{i_3}^\dagger b_{i_1} \rangle = \frac{1}{6N} \sum_k \left[ \frac{\lambda}{\epsilon_1(k)} - \frac{\lambda}{\epsilon_2(k)} \right],
\]
(13)
and \( \langle b_{i_1}^\dagger b_{i_1} \rangle = \langle b_{i_2}^\dagger b_{i_2} \rangle = \langle b_{i_3}^\dagger b_{i_3} \rangle = 1/3 \). Therefore, we find \( \langle S^\alpha \rangle = 0 \) and \( \langle (S^\alpha)^2 \rangle = 2/3 \) \( (\alpha = x, y, z) \), exhibiting that both time reversal and spin rotational symmetries are well preserved in the present MF theory.

Then the spin nematic state with a quadrupole moment \( \langle Q^x \rangle = \langle Q^y \rangle = \langle Q^z \rangle \equiv -Q \) is a possible ground state.

To evaluate the spin spatial correlations in the Mott insulating phase, the dynamic correlation functions should be calculated. By expressing the spin operators in terms of the Nambu spinor, the spin correlations are given by

\[\chi^{\alpha\beta}(q, \omega_m) = \frac{1}{4\beta N} \sum_{k, \omega_n} \text{Tr} \left[ \Gamma_{\alpha} G(k, \omega_n) \Gamma_{\beta} G(k + q, \omega_n + i\omega_m) \right],\]

where \( \Gamma_x, \Gamma_y, \Gamma_z \) denote the corresponding 6 \times 6 matrices of \( S^x, S^y, S^z \); respectively, and both \( \omega_n \) and \( \omega_m \) are bosonic Matsubara frequencies. Inserting the GF matrix and tracing over matrices, we find

\[\chi^{x^z}(q, \omega_m) = \chi^{y^z}(q, \omega_m) = \chi^{z^z}(q, \omega_m),\]

(14)
displaying an SU(2) spin rotational symmetry. The corresponding imaginary part \( \chi^{\alpha_\beta}(q, \omega) \) can also be obtained through performing the summation over the Matsubara frequency and analytic continuation [19].

According to the fluctuation-dissipation theorem, the static spin structure factor is thus obtained \( S_D(q) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega [1 + n_B(\omega)] \chi^{\alpha\beta}(q, \omega) \).

Furthermore, when the correlation function of the quadrupole operator is defined by \( S_Q(\mathbf{r} - \mathbf{r'}) = \langle \{ S^x_{\mathbf{r}} S^y_{\mathbf{r'}} \} / 2 \rangle \), the static quadrupole structure factor \( S_Q(q) \) can be evaluated as well [19].

In 1D, \( z = 2 \) and \( \gamma_k = \cos k \). For a given value of \( J_1/J_2 \), the saddle point equations are solved numerically, results being displayed in Fig.1. For \( 0 \leq J_1/J_2 < 0.19833 \), we find \( \Delta_0 = 0, \Delta_\alpha = 0.5077J_2 \), the quasiparticle band \( \epsilon_1(k) \) and \( \epsilon_2(k) \) are degenerate, so the ground state is a spin singlet with an energy gap. From the point of view of spin correlations, such a spin singlet phase is similar to the spin dimerized state in the limit \( J_1 = 0 \) [17]. For \( J_1/J_2 > 0.19833 \), both \( \Delta_0 \) and \( \Delta_\alpha \) are finite, and two energy gaps in the quasiparticle bands are found

\[
\Delta_{s,1} = \sqrt{\lambda^2 - 4[(3J_2 - J_1)\Delta_\alpha + 2J_1\Delta_0]^2} \quad \text{and} \quad \Delta_{s,2} = \sqrt{\lambda^2 - 4[(3J_2 - J_1)\Delta_\alpha - J_1\Delta_0]^2}
\]
at momenta \( k = 0, \pm \pi \).

Moreover, the quadrupole moment \( Q \) jumps from 0 to 0.16897 at the critical coupling \( J_1/J_2 = 0.19833 \), and then the system is in a short-range ordered spin singlet phase with a finite quadrupole moment. Thus, there is a first-order quantum phase transition from the spin singlet to spin nematic phase with gapful excitations.

If we rewrite \( J_1 = -\cos \theta \) and \( J_2 = -\sin \theta \), the critical coupling corresponds to \( \theta_c = -0.5633\pi \). In fact, a disordered spin nematic (non-dimerized) phase with breaking the SU(2) spin rotational symmetry was first suggested around \( \theta \approx -3\pi/4 \) by Chubukov [12]. However, subsequent numerical work [14] did not support this proposal and it was then believed that the dimerized phase prevails in the whole regime \( -3\pi/4 \leq \theta \leq -\pi/2 \), i.e., \( 0 < J_1/J_2 < 1 \). On the other hand, recent quantum Monte Carlo [20, 21], density matrix renormalization group calculations [22], and quantum field theory approach [22] indicate that the dimerized phase may end at \( \theta \sim -0.67\pi \), casting doubts on the earlier anticipations.

To put our MF results on a solid ground, the static spin structure factor \( S_D(q) \) and quadrupole structure factor \( S_Q(q) \) are calculated at \( T = 0 \)K and displayed in Fig.2. We find that \( S_Q(q) \) exhibits a broad peak around the antiferromagnetic wave vector \( q = \pi \) in both spin singlet and gapped spin nematic phase. However, the quadrupole structure factor \( S_Q(q) \) shows a broad peak around the ferromagnetic wave vector \( q = 0 \) in the spin singlet phase, while \( S_Q(q) \) exhibits a sharp resonance at \( q = 0 \) in the spin nematic phase, indicating strong ferroquadrupolar spatial correlations.

On a 2D square lattice, we have \( z = 4 \) and \( \gamma_k = (\cos k_x + \cos k_y)/2 \). At \( T = 0 \)K, the conversion from summation over momentum to integral will be valid as \( \lambda \rightarrow 4[(3J_2 - J_1)\Delta_\alpha + 2J_1\Delta_0] \), and then the quasiparticle band \( \epsilon_1(k) \) becomes gapless and linear near \( k^* = (0, 0) \) and \( (\pi, \pi) \). The Bose-Einstein condensation thus occurs, while a finite energy gap still exists in the band \( \epsilon_2(k) \). By separating the divergent term from the summation, we can introduce a superfluid density \( \rho_s \) and then solve the saddle point equations. The results are
As a comparison, the calculated static quadrupole structure factor $S_Q(q_x, q_y)$ is displayed in Fig.4b, where a $\delta$-like resonance appears at $q = (0, 0)$, implying strong ferroquadrupolar long-range correlations. These are unique features of an ordered spin nematic phase, which can be directly probed by polarized inelastic light scattering experimentally.

To summarize, the SU(3) boson representation is used to develop an efficient valence bond MF theory for the Mott insulation phase with odd number of spin-1 bosons in optical lattices. A first-order quantum phase transition from a spin singlet to a nematic phase with gapful excitations is predicted for 1D, while on a 2D square lattice a spin nematic ordered phase is shown to always prevail. Both predictions are further supported by an explicit calculation of the spin and quadrupole correlation functions.

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