Spontaneous plaquette formation in the SU(4) Spin-Orbital ladder

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The low-energy properties of the SU(4) spin-orbital model on a two-leg ladder are studied by a variety of analytical and numerical techniques. Like in the case of SU(2) models, there is a singlet-multiplet gap in the spectrum, but the ground-state is two-fold degenerate. An interpretation in terms of SU(4)-singlet plaquettes is proposed. The implications for general two-dimensional lattices are outlined.

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The properties of Mott insulators with orbital degeneracy is attracting a lot of attention with the increasing evidence that this degeneracy can have many other consequences apart from the standard cooperative Jahn-Teller effect. One of the possibilities that seems to be realized in LiNiO\textsubscript{2} is that the additional orbital degree of freedom prevents the system from ordering in both the orbital and spin channels. It was suggested in a recent paper by Li et al.\textsuperscript{[3]} that this might occur if spin and orbital degrees of freedom play a very symmetric role, like in the SU(4) symmetric version of the Kugel'-Khomskii model\textsuperscript{[3]} defined by the Hamiltonian:

\[ H = \sum_{ij} J_{ij}(2\vec{s}_i \cdot \vec{s}_j + \frac{1}{2})(2\vec{\tau}_i \cdot \vec{\tau}_j + \frac{1}{2}) \]  

(1)

Such a Hamiltonian is indeed a good starting point for LiNiO\textsubscript{2} due to the local symmetry and the strong Hund’s rule coupling, but its properties are only beginning to be understood. The fundamental difference with SU(2) models stems from the fact that it takes at least 4 sites to make an SU(4) singlet. For the 1D version of the model, which is fairly well understood both at zero\textsuperscript{[3]}\textsuperscript{[4]}\textsuperscript{[5]}\textsuperscript{[6]} and finite temperature\textsuperscript{[7]}, this shows up as a four-site periodicity of the correlation function. In 2D lattices, it was argued by Li et al.\textsuperscript{[2]}\textsuperscript{[3]} that the system might prefer to form local SU(4) singlet plaquettes in the ground state rather than developing long-range order. While exact diagonalizations (ED) of the model on a square lattice indeed support this conjecture\textsuperscript{[1]}, the lack of analytical results in any limit prevents one from drawing definite conclusions.

As we shall see, exact diagonalizations suggest that the ground state is a two-fold degenerate plaquette solid with gapped multiplet excitations. The important step forward though is that analytical results can be obtained in both the weak and strong rung limits finally putting this plaquette picture on very firm grounds.

The SU(4) spin-orbital model on a ladder is defined by the Hamiltonian

\[ H = J_\parallel \sum_{i,\alpha}(2\vec{s}_{i,\alpha} \cdot \vec{s}_{i+1,\alpha} + \frac{1}{2})(2\vec{\tau}_{i,\alpha} \cdot \vec{\tau}_{i+1,\alpha} + \frac{1}{2}) \]
\[ + J_\perp \sum_{i}(2\vec{s}_{i,1} \cdot \vec{s}_{i,2} + \frac{1}{2})(2\vec{\tau}_{i,1} \cdot \vec{\tau}_{i,2} + \frac{1}{2}), \]

(2)

where a site on the two-leg ladder is described by its rung number \( i \) and its chain index \( \alpha = 1, 2 \), \( \vec{s}_{i,\alpha} \) is a spin one-half operator at site \((i,\alpha)\) and \( \vec{\tau}_{i,\alpha} \) is an isospin one-half corresponding to the orbital degree of freedom on the same site (see Fig. 1).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{The spin-orbital ladder.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2.png}
\caption{Scaling of the singlet-multiplet gap (+) and the singlet-singlet gap (X). The dashed line is a fit with \( \Delta_{sm} = \Delta_{sm}^0 + B N^{-\gamma} \). It is clearly consistent with a non-zero value of \( \Delta_{sm} \) in the \( N \to \infty \) limit, whereas the behavior of \( \Delta_{ss} \) is consistent with a zero value in the same limit.}
\end{figure}

**ISOTROPIC LADDER** – We start by considering the case that is closer to 2D, namely the isotropic limit \( J_\perp = J_\parallel = J \). Taking advantage of all symmetries (translation, rung-parity and SU(4) quantum numbers \( s_{\text{tot}}^z, \tau_{\text{tot}}^z \)
and $s_{\text{tot}}^z = \sum_i s_i^z$, we have obtained the low-energy spectrum on clusters with 8, 12 and 16 sites with Lanczos ED using periodic boundary conditions in the chain direction. The results can be summarized as follows. For all clusters, the ground state is an SU(4) singlet, and the first multiplet excitation is at relatively high energy. Besides, a plot of this energy gap $\Delta_{\text{sm}}$ as a function of $1/N$ (see Fig. 2) strongly suggests that this gap remains in the thermodynamic limit. In addition to this multiplet excitation there is always one low-lying singlet inside this gap (2 in the special case of $N=8$). The splitting between this excited singlet and the ground state $\Delta_s$ is plotted in Fig. 2 as a function of $1/N$. Although it is difficult to draw definite conclusions with only 3 sizes, these results strongly suggest that this gap vanishes, and that the ground state is two-fold degenerate in the thermodynamic limit.

Fig. 3 shows the dispersion of the low-lying states for 16 sites. Two important facts are to be noticed here. First, the ground state and the next singlet lie in the $k = 0$ and $k = \pi$ sectors respectively. Second, the dispersion has a local minimum at $k = \pi/2$, which announces the soft mode at $k = \pi/2$ found in the chain limit where $J_\perp = 0$.

All these results can be qualitatively interpreted in terms of plaquette coverings of the ladder. The plaquette is the ground state of the four-site SU(4) spin-orbital system. It is the smallest SU(4) singlet one can build with a system of degrees of freedom in the fundamental ($d = 4$) representation of SU(4). It undergoes extremely strong fluctuations which minimize the energy by link to $E_0/N = -J$. It is thus a very stable object and can be used to describe the physics of many realizations of this model. For a larger system with $N = 4p$, $p \in \mathbb{N}$, one can build tensor-product states as coverings by such plaquettes in which the system is ‘tetramerized’.

In the case of the two-chain ladder, the number of such plaquette coverings is two, as shown in Fig. 4a. These two coverings differ by a translation by one lattice spacing along the direction of the ladder. They are rung-symmetric, thus having a + rung-parity. A symmetric and an antisymmetric linear combination of these states can be built, giving one $k = 0$ and one $k = \pi$, + rung-parity SU(4) singlet state. These quantum numbers agree with our ED results. In the special case of the $N = 8$ ladder, which has the same topology as a cube, there is an extra covering, corresponding to the third pair of cube faces that can be occupied by each of the two plaquettes (see Fig. 4b). So the plaquette picture predicts 3 low-lying states in this special case, again in agreement with our ED results. Besides, if the ground state is a product of singlet plaquettes, multiplet excitations require the breaking of a plaquette, with a finite energy cost equal to $2J$ minus a correction due to the delocalization of this defect, again in agreement with our ED results.

So all the basic features of our numerical results are qualitatively reproduced by this simple plaquette picture. The following strong coupling approach provides more elements to support this tetramerization picture.

**Strong Coupling** – We now turn to the strong rung limit $J_\perp \gg J_\parallel$. When $J_\parallel = 0$, the ground state is obtained by putting each rung in one of its 6 ground states. The ground state of a rung can be thought of as the set of states (spin singlet $\times$ orbital singlet) and (spin singlet $\times$ orbital triplet) to first order in $J_\perp$, we need only to consider the couplings between two adjacent rungs. Denoting by (12) and (34) the sites of two adjacent rungs, we can actually couple them in two equivalent ways: 1 to 3 and 2 to 4 ($H_1$) or 1 to 4 and 2 to 3 ($H_2$). To first order, the effective Hamiltonians corresponding to $H_1$ and $H_2$ can be formally written:

$$H_{1/2}^{\text{eff}} = \sum_{i,j} |i\rangle V_{ij}^{1,2} \langle j|$$

where the sum over $i, j$ runs over the 36 states of the $J_\parallel = 0$ limit. Now, to go from $H_1^{\text{eff}}$ to $H_2^{\text{eff}}$, we just have to exchange sites 3 and 4. But this transforms any ket $|i\rangle$ (respectively bra $\langle j|$) in the sum of Eq. (3) into $-|i\rangle$.
(respectively $-\langle j|\rangle$ since this permutation just changes the sign of the singlet and leaves the triplet invariant. Given the form of the effective Hamiltonian, we thus have $H^{\text{eff}}_1 = H^{\text{eff}}_2$.

Now the sum of these Hamiltonians $H_0 = H_1 + H_2$ is a very simple operator because each site is coupled to both sites of the opposite rung. In terms of the 15-dimensional vector $\vec{A}$ of each rung, whose components are the generators of $SU(4)$, it can be written

$$H_0 = \frac{J}{4} [\vec{A}_{12} \cdot \vec{A}_{34}] + J'$$

with $\vec{A}_{12} = \vec{A}_1 + \vec{A}_2$ and $\vec{A}_{34} = \vec{A}_3 + \vec{A}_4$. As shown in Ref. [11], this Hamiltonian can be rewritten in terms of Casimir operators as:

$$H_0 = 4J_{||}C_{1234} - 4J_{||}(C_{12} + C_{34}) + J'$$

So the spectrum obtained when coupling two irreducible representations of dimension 6 consists of three levels with degeneracy 1, 15, 20 and with energy $-4(J_{||} + J_\perp)$, $-4J'_{||}$ and $-4(J'_{||} - J_\perp)$ respectively. The spectrum of $H_0$ is thus linear in $J'_{||}$. So $H^{\text{eff}}_0 = H_0$, and since $H^{\text{eff}}_1 = H^{\text{eff}}_2$ and $H_1 + H_2 = H_0$, we reach the conclusion that $H^{\text{eff}}_1 = \frac{1}{2}H_0$.

A more pedestrian way to reach this conclusion consists in calculating the spectrum of $H_1$. For small $J'_{||}$, the levels are linear in $J'_{||}$, and we have checked numerically that the splittings and degeneracies of $H_1$ correspond to $H_0/2$ when $J'_{||}$ is small. Back to the ladder, the first-order Hamiltonian thus writes up to a constant

$$H^{\text{eff}} = \frac{J}{8} \sum_{i,j} \vec{A}_{i,tot} \cdot \vec{A}_{j,tot}$$

where $\vec{A}_{i,tot} = \vec{A}_{i1} + \vec{A}_{i2}$. $H_0$ is thus nothing but the $SU(4)$ Hamiltonian for the $\vec{A}_{i,tot}$ rung degree of freedom. In other words, the effective Hamiltonian is the 1D $SU(4)$ model in the antisymmetric 6-dimensional representation (see Fig. 2). This situation is analogous to going from the $S = 1/2$ $SU(2)$ spin ladder with ferromagnetic rungs to the $S = 1$ $SU(2)$ spin chain.

$$J_0$$

$\times$ $SU(4)$ d=4 IR

$\star$ $SU(4)$ d=6 IR

FIG. 5. (a) The strong-coupling low-energy effective Hamiltonian for the $SU(4)$ spin-orbital ladder. ($\times$) stand for $d = 4$ IR degrees of freedom while ($\star$) stands for $d = 6$ IR degrees of freedom.

This simple form of the effective Hamiltonian has very interesting consequences. The $d = 6$ representation of $SU(4)$ is a self-conjugate and antisymmetric representation of an $SU(N)$ group with $N$ even. It thus falls in the cases where the Lieb-Schultz-Mattis-Affleck theorem states that the $SU(4)$ Hamiltonian should either have a non-degenerate ground-state followed by gapless excitations or have a degenerate ground-state. Affleck, Arovas, Marston and Rabson have shown that the ground-state is a two-fold degenerate singlet, and breaks translation invariance. More precisely, the two ground-states are spontaneously dimerized, nearest-neighboring sites forming $SU(4)$ singlets either between neighbors $(2n, 2n+1)$ or between neighbors $(2n+1, 2n+2)$. Above these ground states there is a gap to magnon-like or soliton-like excitations [13,14]. DMRG calculations confirmed this picture of dimer-order with short-range spin-spin correlations ($\vec{A}$-spin correlation length of the order of the lattice spacing).

This strong-coupling regime is very similar to the physics we have characterized numerically in the intermediate coupling regime and strongly supports our plaquette interpretation. First of all, the spectrum has the same properties in both cases: The two plaquette-states break translation symmetry, have a short correlation length, and the first excitation has to be built breaking one plaquette, thus leading to a gap. Besides, a tetramerization of a ladder is equivalent to a dimerization in terms of rungs. We now come to the weak-coupling regime to show how the situation sets in when two $SU(4)$ gapless chains are coupled to form a ladder.

**Weak Coupling** – The weak-coupling approach proceeds in an analogous way as in the $SU(2)$ ladder. In the absence of interchain coupling ($J_\perp = 0$) the Hamiltonian (1) describes two decoupled $SU(4)$ spin chains and is exactly solvable by the Bethe ansatz [4]. The system is gapless and the low energy physics is described by six (three for each chain) massless bosons and is controlled by the fixed point Hamiltonians of two decoupled Wess-Zumino-Novikov-Witten (WZNW) $SU(4)$ models [2] with central charge $c = 3+3 = 6$. As in the $SU(2)$ ladder, the strategy to tackle with the weak coupling regime is to look at the stability of the infrared fixed point with respect to the interchain coupling. To this end one needs the low energy expressions for the $SU(4)$ spin densities in terms of the WZNW fields which has been obtained in Refs. [17]

$$S_a^A = J_{aKL} + J_{aL} + \left[ e^{i\pi/2} N_a^A + H.c. \right] + (-1)^{x/\pi} a_a^A$$

where $S_a^A$ are the 15 $SU(4)$ spin densities of chain index $a = 1, 2$ with components $J_{aKL}^A$ at $k = 0$, $N_a^A$ at $2k_F = \pi/2$, and $n_a^A$ at $4k_F = \pi/4$. The uniform part of the spin density is the $SU(4)$ spin current with scaling dimension $d_0 = 1$. The other oscillating parts, $N_a^A$ and $n_a^A$ are WZNW primary fields with scaling dimensions...
Coupled SU(4) spin ladder obtain the low energy effective Hamiltonian of the weakly coupled SU(4) spin ladder

\[ \mathcal{H}_{\text{eff}} = \frac{2\pi v}{5} \sum_{a=1}^{2} (J_{aR}^{A} J_{aL}^{A} + (R \to L)) \]
\[ + J_{\perp} (J_{1R}^{A} J_{2L}^{A} + J_{1L}^{A} J_{2R}^{A} + n_{1}^{A} n_{2}^{A}) \]
\[ + J_{\perp} \left( \mathcal{N}_{1}^{A} \mathcal{N}_{2}^{A} + \mathcal{N}_{1}^{A} \mathcal{N}_{2}^{A} \right), \]

where we have dropped as usual the marginally irrelevant current-current in-chain interactions as well as the interaction between the current of the two chains with the same chirality that renormalizes the spin velocity. The interacting part of Eq. (8) has two contributions. One comes from the uniform and \( 4k_F \) parts of the spin densities (6). It is marginal with scaling dimension 2. The other contribution, which stems from the \( 2k_F \) spin densities, is in a strongly relevant perturbation with scaling dimension 3/2 and thus governs the low energy behavior of the model. As an immediate consequence we conclude that a gap \( \Delta \sim J_{\perp}^{2} \) opens in the spectrum. The delicate point however is whether or not some gapless modes survive in the infrared. This issue can be investigated by means of the Abelian bosonization of the SU(4) spin densities (6). Using the results of Ref. [17] we have expressed the effective Hamiltonian (8) in terms of the six bosonic fields that describe the ultraviolet fixed point. The resulting bosonized Hamiltonian is too lengthy to be reproduced here but it can be shown that all degrees of freedom are massive.

At this point, the physically relevant question is whether the “plaquette” picture drawn from the strong coupling analysis survives at weak coupling, and in particular whether the nature of the low lying excitations at strong coupling changes as the interchain coupling is reduced. In the SU(2) ladder, the nature of the low energy spectrum is the same in both limits and is captured by the weak coupling approach. In this case it has been shown in Ref. [18] that the effective Hamiltonian separates into two decoupled free field theories (free massive real fermions) that describe both singlet and triplet sectors. In contrast in the SU(4) model an analogous decomposition does not hold. Indeed, the leading part of the bosonized Hamiltonian does not split into two parts that account for the six-dimensional (antisymmetric) and tenth-dimensional (symmetric) SU(4) irreducible representation: All degrees of freedom strongly interact. In the simplest hypothesis, we expect that no phase transition occurs between weak and strong couplings but rather a smooth cross-over to the plaquette picture described above.

**Conclusion** – In summary, coming back to the issue raised in the introduction, we now have definite evidence that the presence of an SU(4) symmetry can indeed have very dramatic consequences for lattices in which plaquettes can form. In the case of the two-leg ladder we have shown that there is a spontaneous plaquette formation that leads to a degenerate singlet ground state in an otherwise gapped spectrum. This leads naturally to the conjecture that, for more general lattices, there will be low lying singlets, and that such plaquette coverings provide a good variational basis to describe them. Work is in progress along these lines.

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