One-Dimensional SU(4) Spin-Orbital Model: A Low-Energy Effective Theory

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The one-dimensional spin-orbital model is studied by means of Abelian bosonization. We derive the low-energy effective theory which enables us to study small deviations from the SU(4) symmetric point. We show that there exists a massless region with algebraically decaying correlation functions $\sim \cos[(\pi/2a_0)x]x^{-3/2}$. When entering the massive phase, the system displays an approximate SO(6) enlarged symmetry with a dimerization type of ordering consisting in alternating spin and orbital singlets.

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The interest in spin-orbital models stems from the possibility of understanding the magnetic structures of transition metal compounds [1]. In most of these materials, in addition to the usual spin degeneracy, the low-lying electron states are also characterized by orbital degeneracy. It is thus believed that the unusual magnetic properties observed in many of these compounds should be explained in terms of simple multiband Hubbard-like models. Very recently, the discovery of new spin-gapped materials, $Na_2Ti_2Sb_2O$ [2] and $Na_2V_2O_5$ [3], has attracted renewed interest in the spin-orbital models. These materials have a quasi-1D structure [4] and are modeled by a quarter-filled *two*-band Hubbard model which, in the limit of strong Coulomb repulsion, is equivalent to two interacting Heisenberg models with the Hamiltonian:

$$\mathcal{H} = \sum_i J_1 \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \vec{T}_i \cdot \vec{T}_{i+1} + K(\vec{S}_i \cdot \vec{S}_{i+1})(\vec{T}_i \cdot \vec{T}_{i+1}), \quad (1)$$

where $\vec{S}_i$ and $\vec{T}_i$ are spin-1/2 operators representing the spin and orbital degrees of freedom at each site i, and $J_{1,2}$ and K are positive constants.

The Hamiltonian (1) is invariant under independent SU(2) rotations in the spin ($\vec{S}$) and orbital ($\vec{T}$) spaces. It can also be recast as a two-leg spin ladder with a four-spin interchain coupling. In the limit $K \ll J_{1,2}$ this interaction, which can be generated either by phonons or (in the doped state) by the Coulomb repulsion between the holes, gives rise to a non-Haldane spin-liquid state where magnon excitations are incoherent [5]. The physically relevant question is whether or not this scenario can be extended to larger values of K for which (1) is expected to be of experimental relevance.

As a matter of fact, we already know that this cannot be the case. Indeed, the interesting feature of the Hamiltonian (1) is that at $J_1 = J_2 = K/4$ it is not only SU(2) $\times$ SU(2) symmetric but actually has an enlarged SU(4) symmetry [6]. At this special point, the model is Bethe-ansatz solvable [7] and critical with *three* gapless bosonic modes; in the conformal field theory language, that means that the central charge is $c = 3$ and, as shown by Affleck [8], the critical theory corresponds to the $SU(4)_1$ Wess-Zumino-Novikov-Witten (WZNW) model. Clearly, there should be a *qualitative* change in the physical behavior of (1) when going from small to large values of K. From the theoretical point of view, this situation is striking because it implies that one cannot go continuously from weak to strong coupling. This is a manifestation of Zamolodchikov's c theorem which states that, starting at $K = 0$ with two decoupled S $= 1/2$ Heisenberg chains with the total central charge $c = 2$ (two gapless bosons), one cannot flow—in the renormalization group (RG) sense—towards the SU(4) point which has a larger central charge $c = 3$. Therefore, the physics in the neighborhood of the SU(4) point cannot be understood in terms of weakly coupled Heisenberg chains, and the general strategy employed to tackle spin ladders does not apply here: A new effective theory is to be developed. It is the purpose of this work to do so. Below, we present an effective continuum description of the model (1) at the SU(4) point, based on Abelian bosonization, and derive the low-energy expressions for the spin and orbital densities. With these results at hand, we then investigate the properties of differing phases occurring at small deviations from the SU(4) point.

Abelian bosonization at the SU(4) point.—We start by introducing the SU(4) Hubbard model with $U > 0$:

$$\mathcal{H}_U = \sum_{ia\sigma} (-t c^\dagger_{i+1a\sigma} c_{ia\sigma} + \text{H.c.}) + \frac{U}{2} \sum_{iab\sigma\sigma'} n_{ia\sigma} n_{ib\sigma'} (1 - \delta_{ab}\delta_{\sigma\sigma'}). \quad (2)$$

Here, $c^\dagger_{ia\sigma}$ creates an electron with the "flavor" (orbital) index $a = 1,2$ and spin $\sigma = \uparrow, \downarrow$, and $n_{ia\sigma} = c^\dagger_{ia\sigma} c_{ia\sigma}$. It will be assumed that the electron band is quarter-filled implying that the Fermi momentum $k_F = \pi/4a_0$, where a_0 is the lattice spacing. The spin and orbital operators are defined as

$$\vec{S}_i = \frac{1}{2}\sum_a c^\dagger_{ia\alpha}\vec{\sigma}_{\alpha\beta}c_{ia\beta}, \qquad \vec{T}_i = \frac{1}{2}\sum_\alpha c^\dagger_{ia\alpha}\vec{\tau}_{ab}c_{ib\alpha}\,, \tag{3}$$

where $\vec{\sigma}$ ($\vec{\tau}$) are the Pauli matrices acting in the spin (orbital) space.

The low-energy physics can be described in terms of right-moving ($R_{a\sigma}$) and left-moving ($L_{a\sigma}$) fermions which replace the original lattice fermion $c_{ia\alpha}$ in the continuum limit ($x = ia_0$):

$$\frac{c_{ia\sigma}}{\sqrt{a_0}} \simeq R_{a\sigma}(x)\exp(\mathrm{i}k_F x) + L_{a\sigma}(x)\exp(-\mathrm{i}k_F x)\,. \tag{4}$$

At this point, we introduce four chiral bosonic fields $\Phi_{a\sigma R,L}$ using Abelian bosonization of Dirac fermions: $R(L)_{a\sigma} = \kappa_{a\sigma}(2\pi a_0)^{-1/2}\exp(\pm\mathrm{i}\sqrt{4\pi}\,\Phi_{a\sigma R(L)})$. The bosonic fields satisfy the commutation relation $[\Phi_{a\sigma R}, \Phi_{b\sigma' L}] = \frac{i}{4}\delta_{ab}\delta_{\sigma\sigma'}$. Anticommutation between the fermions with different spin-channel indices is ensured by Klein factors (here Majorana fermions) $\kappa_{a\sigma}$. It is then suitable to employ a physically transparent basis (cf. Ref. [9]):

$$\begin{aligned}
\Phi_c &= (\Phi_{1\uparrow} + \Phi_{1\downarrow} + \Phi_{2\uparrow} + \Phi_{2\downarrow})/2\,,\\
\Phi_s &= (\Phi_{1\uparrow} - \Phi_{1\downarrow} + \Phi_{2\uparrow} - \Phi_{2\downarrow})/2\,,\\
\Phi_f &= (\Phi_{1\uparrow} + \Phi_{1\downarrow} - \Phi_{2\uparrow} - \Phi_{2\downarrow})/2\,,\\
\Phi_{sf} &= (\Phi_{1\uparrow} - \Phi_{1\downarrow} - \Phi_{2\uparrow} + \Phi_{2\downarrow})/2\,.
\end{aligned} \tag{5}$$

In the new basis, the total charge degree of freedom is described by Φ_c, while the non-Abelian (spin-orbital) degrees of freedom are faithfully represented by three bosonic fields Φ_a ($a = s, f, sf$). It is now straightforward to obtain the continuum limit of the Hubbard Hamiltonian (2) which exhibits separation between the charge and spin-orbital parts of the spectrum. The charge sector is described by a Gaussian model for the field Φ_c perturbed by an umklapp term $\sim\cos\sqrt{16\pi K_c}\,\Phi_c$ generated in higher orders of perturbation theory. Though at small U the umklapp term is irrelevant and the charge excitations remain gapless, one expects that on increasing the Coulomb interaction the nonuniversal parameter $K_c(U)$ will decrease and eventually reach the critical value $K_c(U_c) = 1/2$ where a Mott transition occurs to an insulating phase [8,12]. Though one certainly expects the system to be insulating in the limit $U/t \to \infty$ [1,10,11], the question whether a commensurability gap, m_c, opens at a *finite* value of U is beyond the scope of perturbation theory. Very recently, Assaraf *et al.* [12] using an improved Monte Carlo method were able to show that there exists a critical value $U = U_c \sim 2.8t$ above which $m_c \neq 0$. Assuming $U > U_c$, in what follows we shall focus on the spin-orbital sector described by the Hamiltonian:

$$\begin{aligned}
\mathcal{H}_{\rm so} = &\sum_{a=s,f,sf}\left\{\frac{v_F}{2}[(\partial_x\Phi_a)^2 + (\partial_x\Theta_a)^2] + \frac{G_3}{\pi}(\partial_x\Phi_a)^2\right\}\\
&- \frac{G_3}{\pi^2 a_0^2}\sum_{a\neq b}\cos\sqrt{4\pi}\,\Phi_a\cos\sqrt{4\pi}\,\Phi_b\,,
\end{aligned} \tag{6}$$

where $G_3 = -Ua_0/2$, and $\Theta_a = \Phi_{aL} - \Phi_{aR}$ are the fields dual to Φ_a. The structure of the last term in (6) immediately suggest refermionization of the three bosonic fields Φ_a in terms of six real (Majorana) fermions ξ^a, $a = (1, \ldots, 6)$:

$$\begin{aligned}
(\xi^1 + \mathrm{i}\xi^2)_{R(L)} &= \frac{\eta_1}{\sqrt{\pi a_0}}\exp(\pm\mathrm{i}\sqrt{4\pi}\,\Phi_{sR(L)})\,,\\
(\xi^3 + \mathrm{i}\xi^4)_{R(L)} &= \frac{\eta_2}{\sqrt{\pi a_0}}\exp(\pm\mathrm{i}\sqrt{4\pi}\,\Phi_{fR(L)})\,,\\
(\xi^5 + \mathrm{i}\xi^6)_{R(L)} &= \frac{\eta_3}{\sqrt{\pi a_0}}\exp(\pm\mathrm{i}\sqrt{4\pi}\,\Phi_{sfR(L)})\,,
\end{aligned} \tag{7}$$

η_i being another Klein factor. In this representation the original SU(4) transformations of the complex fermion fields appear as SO(6) rotations on the Majorana sextet $\{\xi^a\}$, reflecting the equivalence SU(4) $\sim$ SO(6). To get a better insight in the symmetry properties of our model, let us define the spin and orbital triplets: $\vec{\xi}_s = (\xi^2, \xi^1, \xi^6)$ and $\vec{\xi}_t = (\xi^4, \xi^3, \xi^5)$. Those transform as vectors under spin $\mathrm{SO}(3)_s$ and orbital $\mathrm{SO}(3)_t$ rotations, respectively. In the Majorana representation, the Hamiltonian (6) reduces to an SO(6) Gross-Neveu (GN) model:

$$\mathcal{H}_{\rm so} = -\frac{iv_s}{2}\sum_{a=1}^{6}(\xi^a_R\partial_x\xi^a_R - \xi^a_L\partial_x\xi^a_L) + G_3\left(\sum_{i=1}^{6}\kappa_i\right)^2, \tag{8}$$

with $\kappa_i = \xi^i_R\xi^i_L$. Since $G_3 < 0$, we conclude that the interaction term in (8) is marginally irrelevant and the model flows towards six decoupled massless real fermions. Thus, at the fixed point ($G_3^* = 0$), the spin-orbital sector is described by the $\mathrm{SO}(6)_1$ [$\sim\mathrm{SU}(4)_1$] WZNW model with the central charge $c = 6 \times 1/2 = 3$.

To complete our description of the SU(4)-symmetric critical point, we present the continuum expressions for the effective spin and orbital densities:

$$\begin{aligned}
\vec{S} &= \vec{J}_{sR} + \vec{J}_{sL} + \exp(\mathrm{i}\pi x/2a_0)\vec{\mathcal{N}}_s + \mathrm{H.c.} + (-1)^{x/a_0}\vec{n}_s\,,\\
\vec{T} &= \vec{J}_{tR} + \vec{J}_{tL} + \exp(\mathrm{i}\pi x/2a_0)\vec{\mathcal{N}}_t + \mathrm{H.c.} + (-1)^{x/a_0}\vec{n}_t\,,
\end{aligned} \tag{9}$$

Here $\vec{J}_{s,t}$ are the smooth ($k \sim 0$) parts of these densities, while $\vec{\mathcal{N}}_{s,t}$ and $\vec{n}_{s,t}$ are the $2k_F = \pi/2a_0$ and $4k_F = \pi/a_0$ parts. Notice that Eqs. (9) have a more complicated structure than that of the spin density in the usual Hubbard model. The emergence of $4a_0$ oscillations and the corresponding complex fields $\vec{\mathcal{N}}_{s,t}$ is a consequence of the band's quarter-filling. The smooth and $2k_F$ contributions can be computed directly from Eqs. (3). We find that the chiral vector currents,

$$\vec{J}_{sR(L)} = -\frac{\mathrm{i}}{2}\,\vec{\xi}_{sR(L)} \wedge \vec{\xi}_{sR(L)}\,,$$

$$\vec{J}_{tR(L)} = -\frac{\mathrm{i}}{2}\,\vec{\xi}_{tR(L)} \wedge \vec{\xi}_{tR(L)}\,,$$

are in fact $SU(2)_2$ currents, in contrast with a single Heisenberg chain where the smooth part of the spin density is a sum of $SU(2)_1$ vector currents. The fields $\vec{\mathcal{N}}_{s,t}$ are nonlocal in the Majorana fermions $\vec{\xi}_{s,t}$. However, as in the two-leg ladder problem [13], they acquire a local form when expressed in terms of order and disorder operators σ_a and μ_a of the six critical Ising models associated with the six Majorana fermions. The expressions of $\vec{\mathcal{N}}_{s,t}$ are manifestly $SO(3)_{s,t}$ invariant; here we give only their z components: $\mathcal{N}_s^z = A(\mathrm{i}\mu_1\mu_2\sigma_3\sigma_4\sigma_5\sigma_6 + \sigma_1\sigma_2\mu_3\mu_4\mu_5\mu_6)$ and $\mathcal{N}_t^z = A(\mathrm{i}\sigma_1\sigma_2\mu_3\mu_4\sigma_5\sigma_6 + \mu_1\mu_2\sigma_3\sigma_4\mu_5\mu_6)$, where A is a nonuniversal constant. At the critical point, the order and disorder operators have scaling dimension $1/8$, so the $2k_F$ densities $\vec{\mathcal{N}}_{s,t}$ have dimension $3/4$. Since the $\vec{S}$ and $\vec{T}$ densities involve fermionic bilinears, it may appear surprising to find $4k_F$ contributions $\vec{n}_{s,t}$. However, nothing prevents higher harmonics to be generated in interacting systems. The structure of $\vec{n}_{s,t}$ can be anticipated by symmetry arguments: These fields should be chirally invariant and transform as vectors under $SO(3)_{s,t}$ rotations. These requirements lead to the following simple expressions: $\vec{n}_s = \mathrm{i}B\vec{\xi}_{sR} \wedge \vec{\xi}_{sL}$ and $\vec{n}_t = \mathrm{i}B\vec{\xi}_{tR} \wedge \vec{\xi}_{tL}$ where B is another nonuniversal constant. The scaling dimension of the $\vec{n}_{s,t}$ fields is 1.

Deviations from the SU(4) point.—We are now in a position to investigate the properties of the model (1) at small deviations from the SU(4) point. We shall restrict consideration to symmetric perturbations, $J_1 = J_2 = K/4 + G$, $|G| \ll K$, and postpone the study of a more general case to a future publication. Using the low-energy representation of the spin-orbital densities, one can expand (1) around the $SO(6)_1$ fixed point to find

$$\mathcal{H} = -iu/2(\vec{\xi}_{sR}\cdot\partial_x\vec{\xi}_{sR} - \vec{\xi}_{sL}\cdot\partial_x\vec{\xi}_{sL}) - iu/2(\vec{\xi}_{tR}\cdot\partial_x\vec{\xi}_{tR} - \vec{\xi}_{tL}\cdot\partial_x\vec{\xi}_{tL}) + G_3(\kappa_1+\kappa_2+\kappa_3+\kappa_4+\kappa_5+\kappa_6)^2 + G[(\kappa_1+\kappa_2+\kappa_6)^2 + (\kappa_3+\kappa_4+\kappa_5)^2]. \qquad (10)$$

The Hamiltonian (10) describes two SO(3)-symmetric, marginally coupled, spin and orbital GN models. The G term breaks $SU(4) \sim SO(6)$ symmetry down to $SO(3)_s \otimes SO(3)_f$. Notice that all interactions are marginal. This is the reason why we have also kept the marginally irrelevant (G_3) term which is already present at the SU(4) point [Eq. (8)]. The emerging picture is to be opposed to the case of two weakly coupled Heisenberg chains where the interchain interaction $J_\perp$ gives rise to a strongly relevant perturbation (of scaling dimension 1) and thus opens a spectral gap at arbitrarily small $J_\perp$ [5]. The RG equations for the couplings in (10) are easily obtained at the one-loop level:

$$\dot{G} = G^2 - 2GG_3, \qquad \dot{G}_3 = 4G_3(G + G_3)\,. \qquad (11)$$

The flow analysis reveals the existence of three different regions: A, B, and C, shown in Fig. 1.

In the region B, all couplings are irrelevant and a model with initial conditions in B flows towards the $SO(6)_1$ fixed point. The system is critical and the correlation functions $\mathcal{G}(x,\tau) = \langle\vec{S}(x,\tau)\cdot\vec{S}(0,0)\rangle = \langle\vec{T}(x,\tau)\cdot\vec{T}(0,0)\rangle$ display a power law behavior. In the long distance limit, $\mathcal{G}(x,\tau)$ is dominated by the contributions at $k = 0$, $k = 2k_F$, and $k = 4k_F$:

$$\mathcal{G}_0(x,\tau) \sim -\frac{3}{4\pi^2}[(x + \mathrm{i}u\tau)^{-2} + (x - \mathrm{i}u\tau)^{-2}],$$

$$\mathcal{G}_{\pi/2}(x,\tau) \sim A^2\cos\left(\frac{\pi}{2a_0}x\right)(x^2 + u^2\tau^2)^{-3/4}, \qquad (12)$$

$$\mathcal{G}_\pi(x,\tau) \sim (-1)^{x/a_0}B^2(x^2 + u^2\tau^2)^{-1},$$

the leading asymptotics thus being $\mathcal{G}_{\pi/2}$. In the regions A and C, the interaction is relevant and leads to the dynamical generation of a mass gap. In the far infrared limit, all trajectories flow towards the asymptote L: $G = -2G_3$. There the interacting part Hamiltonian (10) transforms to

$$\mathcal{H}_{\mathrm{int}} = G/2(\kappa_1 + \kappa_2 + \kappa_6 - \kappa_3 - \kappa_4 - \kappa_5)^2. \qquad (13)$$

Upon the transformation $\vec{\xi}_{tR(L)} \to \pm\vec{\xi}_{tR(L)}$, the interaction (13) is easily seen to acquire an SO(6) symmetric form. However, the conclusion that the SO(6) symmetry is restored in both phases A and C would be incorrect. The scaling portrait in phase C is similar to the crossover sector of the Kosterlitz-Thouless phase diagram for the U(1)-symmetric Thirring model where an exact (Bethe-ansatz) solution [14] confirms restoration of SU(2) up to exponentially small corrections. Using arguments given recently by Azaria *et al.* [15], we therefore expect that restoration of SO(6) is a specific feature of phase C, while in the massive region A the nature of elementary excitations is more complicated reflecting the existence of several energy scales. The development of the

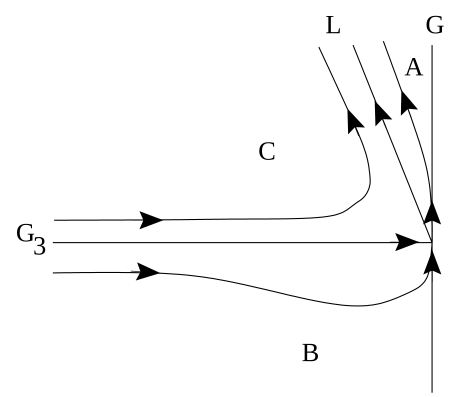

FIG. 1. Flow diagram for isotropic couplings.

strong-coupling regime in the SO(6) GN model, describing phase C, leads to generation of a fermionic mass. As a consequence, $\langle \kappa_{1,2,6} \rangle = -\langle \kappa_{3,4,5} \rangle \neq 0$, indicating spontaneous breakdown of translational invariance. Indeed, the dimerization operators for each chain, $\Delta_s = (-1)^i \vec{S}_i \cdot \vec{S}_{i+1}$ and $\Delta_t = (-1)^i \vec{T}_i \cdot \vec{T}_{i+1}$, express in terms of the energy densities of the two SO(3) spin and orbital GN models: $\Delta_s \sim \kappa_1 + \kappa_2 + \kappa_6$ and $\Delta_t \sim \kappa_3 + \kappa_4 + \kappa_5$. Therefore $\langle \Delta_s \rangle = -\langle \Delta_t \rangle = \pm \Delta_0$, and the system orders in one of two, doubly degenerate, ground states with alternating spin and orbital singlets, in agreement with the weak coupling results [5].

Calculating the exact dynamical correlation functions in the massive phases is difficult. While hopeless in the broken-symmetry phase A, this task could be accomplished in principle in the symmetry-restored phase C since the SO(6) GN model is integrable. The full treatment which takes into account the Z_2 degeneracy of the ground state and the existence of topological (kink) excitations in addition to the fundamental fermion will be presented elsewhere. However, since the mass of the fermion is smaller than twice the kink mass, we expect that fermions will dominate at sufficiently low energy. Their contribution to the correlation functions can be estimated by a mean field approach:

$$\begin{aligned} \langle \vec{S}(x,\tau) \cdot \vec{S}(y,0) \rangle &\sim A^2 \cos\left(\frac{\pi}{2a_0} x\right) \cos\left(\frac{\pi}{2a_0} y\right) K_0(MR) \\ &\quad - (-1)^{x/a_0} B^2 K_0^2(MR)\,, \\ \langle \vec{T}(x,\tau) \cdot \vec{T}(y,0) \rangle &\sim A^2 \sin\left(\frac{\pi}{2a_0} x\right) \sin\left(\frac{\pi}{2a_0} y\right) K_0(MR) \\ &\quad - (-1)^{x/a_0} B^2 K_0^2(MR)\,, \end{aligned} \tag{14}$$

where $R = \sqrt{(x-y)^2 + u^2\tau^2}$ and $K_0(MR)$ is the real space propagator of a free massive fermion. We observe that, on top of an *incoherent* background at $k \sim \pi$ (with weight $\sim B^2$), there is a *coherent* magnon peak at $k = \pi/2$ (with weight $\sim A^2$). This is to be contrasted with the situation at weak coupling ($K \ll J$) where only incoherent magnons at $k \sim \pi$ exist [5]. At this point, it is worth commenting on the status of the nonuniversal parameters A and B that enter in the expressions of the spin densities. The numerical results [11,16] at the SU(4) symmetric point are in good agreement with the expressions (12). In particular, these results have revealed that the peak in the static susceptibility at $2k_F$ is much greater than the one at $4k_F$, thus suggesting that $A \gg B$ at the SU(4) point. This is not to be the case when one deviates from the SU(4) symmetric point, and the question that naturally arises is how, as K decreases, one will move from strong to weak coupling regimes. Since our solution for large K captures the properties of both regimes, it is natural to make the hypothesis that the crossover is encoded in the K dependence of the nonuniversal constants A and B. In the simplest scenario, one may conjecture that $B(K)$ will increase as K decreases while $A(K)$ should decrease. Since A is found to be zero at weak coupling, one may further suspect that it will vanish for K smaller than a critical value K_D. Such a special point where some oscillating component of the correlation function vanishes is called a disorder point [17].

Let us conclude, comparing our results with the recent numerical calculations by Pati *et al.* [4]. Our result for the phase B is in agreement with the numerical data. In the phase C these authors find a doubly degenerate ground state which forms alternating spin and orbital singlets, in agreement with our results. However, they conclude that the mass gap opens with an exponent $\sim 1.5 \pm 0.25$, whereas the bosonization approach predicts that the gap is exponentially small with the deviation from the SU(4) symmetric point. Moreover, they interpret their data in favor of *incommensurate* correlations in contrast with (14). In the continuum approach, we found no room for incommensuration since the parity breaking ("twist") term $i\vec{\mathcal{N}}_a(x + a_0) \cdot \vec{\mathcal{N}}_a^{\dagger}(x)$ + H.c., which appears upon deviating from the critical SU(4) point and which might be a potential source of incommensurations [18], turns out to be irrelevant (with dimension 3). Our result supports another scenario in which the correlation functions contain components at $k \sim 0$, π and $\pi/2$, with amplitudes depending on K.

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