



Zhang, G.-M., Hu, H., & Yu, L. (2003). Spin-orbital gapped phase with least symmetry breaking in the one-dimensional symmetrically coupled spin-orbital model.

Originally published in *Physical Review B: Condensed Matter and Materials Physics*, 67(6).
Available from: <http://dx.doi.org/10.1103/PhysRevB.67.064420>.

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Spin-orbital gapped phase with least symmetry breaking in the one-dimensional symmetrically coupled spin-orbital model

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(February 2, 2008)

Abstract

To describe the spin-orbital energy gap formation in the one-dimensional symmetrically coupled spin-orbital model, we propose a simple mean field theory based on an $SU(4)$ constraint fermion representation of spins and orbitals. A spin-orbital gapped phase is formed due to a marginally relevant spin-orbital valence bond pairing interaction. The energy gap of the spin and orbital excitations grows extremely slowly from the $SU(4)$ symmetric point up to a maximum value and then decreases rapidly. By calculating the spin, orbital, and spin-orbital tensor static susceptibilities at zero temperature, we find a crossover from coherent to incoherent magnetic excitations as the spin-orbital coupling decreasing from large to small values.

PACS Numbers: 75.10.Jm, 75.10.Lp, 75.40.Gb

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It is a very interesting problem to look for exotic quantum magnetic states realized with the spin and orbital degrees of freedom. Since the discovery of new quasi-one-dimensional spin gapped materials $\text{Na}_2\text{Ti}_2\text{Sb}_2\text{O}$ [1] and NaV_2O_5 [2], there has been considerable interest in magnetic systems with orbital degeneracy [3–10]. It is believed that the unusual magnetic properties observed in these compounds can be explained by a simple two-band Hubbard model at quarter filling, and in the large Coulomb repulsion limit the effective Hamiltonian is simplified to a model of two symmetrically coupled spin -1/2 Heisenberg chains: [11–13]

$$H = J \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \mathbf{T}_i \cdot \mathbf{T}_{i+1}) + V \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{T}_i \cdot \mathbf{T}_{i+1}), \quad (1)$$

where \mathbf{S}_i and \mathbf{T}_i denote the spin and orbital degrees of freedom, respectively. Here both coupling parameters J and V are assumed to be antiferromagnetic, and the model Hamiltonian is $\text{SU}(2) \otimes \text{SU}(2)$ symmetric with an additional Z_2 symmetry in exchange between \mathbf{S}_i and \mathbf{T}_i .

For this model, the critical point $V = 0$ describes two independent isotropic Heisenberg spin-1/2 chains with gapless excitations. In the weak coupling regime $V/J \ll 1$, it has been shown that the model describes a non-Haldane spin liquid where magnetic excitations are gapful but *incoherent* [14]. In the strong coupling regime [15] $V/J \gg 1$, however, a special point $V/J = 4$ has been identified where the Hamiltonian becomes $\text{SU}(4)$ invariant [13], and it has been demonstrated by Bethe ansatz and effective field theory methods that the low-energy excitations are *coherent*, given by three branches of gapless elementary excitations [16,17]. However, as emphasized in Ref. [6], there is no renormalization group flow from the first to the second critical points due to the Zamolodchikov theorem on the central charge. In the Heisenberg limit ($V = 0$), the total central charge is $c = 2$, while $c = 3$ at the $\text{SU}(4)$ symmetric point. This means a gapped phase is expected in-between the weak and strong coupling limits with gapless magnetic excitations. In particular, it has been shown [18] that when $V/J = 4/3$, the model has an exact ground state in which spin and orbital operators may form dimerized singlets in a staggered pattern, and such a matrix product state is doubly degenerate and gapped. However, so far it is not clear whether such staggered dimerized singlets can represent the ground state in the whole gapped phase. On the other hand, a crossover transition from incoherent to coherent magnetic excitations is speculated as the spin-orbital coupling changing from small to large values within the gapped phase [6]. Since the perturbation treatment from either end can not provide a unified description, a non-perturbative interpolation scheme would be highly desirable.

The purpose of the present paper is to develop a simple mean field (MF) theory based on the strong-coupling $\text{SU}(4)$ symmetric limit and to describe such a spin-orbital gap formation along with the coherent-incoherent crossover of magnetic excitations. When $V/J < 4$ and is close to the strong-coupling $\text{SU}(4)$ point, the spin and orbital static susceptibilities display very sharp coherent magnon peaks at the nesting wave vector $2k_F = \pi/2$, corresponding to a commensurate spin-density wave of period four lattice spacings. Away from the strong coupling symmetric point, a spin-orbital valence bond (VB) pairing interaction is present, leading to an energy gap in the quasiparticle excitations. The energy gap initially grows *extremely slowly* from $V/J = 4$ up to a maximum value near $V/J \sim 1.265$, and then decreases rapidly to a very small value near $V/J \sim 0.462$. From the calculated spin and orbital static

susceptibilities, the coherent magnetic peaks around $q = \pm\pi/2$ are gradually suppressed and *slightly* shifted, and their spectral weights are transferred to the incoherent background around $q = \pm\pi$. Moreover, the present MF theory also provides the correlation spectra of the spin-orbital tensor operators, exhibiting further clear evidence of the nontrivial crossover from the weak to strong coupling limits of the model.

First, up to a constant, the model Hamiltonian can be rewritten as:

$$H = J_c \sum_i \left(2\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{2} \right) \left(2\mathbf{T}_i \cdot \mathbf{T}_{i+1} + \frac{1}{2} \right) - J_s \sum_i \left(2\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{2} \right) \left(2\mathbf{T}_i \cdot \mathbf{T}_{i+1} - \frac{1}{2} \right), \quad (2)$$

where the first part corresponds to an SU(4) spin-orbital symmetric model in the SU(4) *fundamental* representation [4–7,10], while the second part corresponds to a *staggered* SU(4) spin-orbital VB model [19–21,10] in which alternating sublattice sites transform according to the SU(4) fundamental and anti-fundamental representations, respectively. Here the coupling parameters are regrouped into $J_c = (J/2 + V/8)$ and $J_s = (J/2 - V/8)$.

In the strong coupling SU(4) symmetric point, $V/J = 4$, $J_c = J$ and $J_s = 0$. Our MF theory will take this limit as a starting point, while the weak coupling limit $V = 0$ corresponds to the case of $J_c = J_s = J/2$. In order to maintain the higher symmetry of the strong coupling limit and to characterize both spin and orbital degrees of freedom at the same time, an SU(4) constrained fermion representation is introduced, and its generators are given by $F_\beta^\alpha(i) = C_{i,\alpha}^\dagger C_{i,\beta}$, satisfying the SU(4) Lie algebra

$$[F_\beta^\alpha(i), F_\nu^\mu(i)] = \delta_{\beta,\mu} F_\nu^\alpha(i) - \delta_{\alpha,\nu} F_\beta^\mu(i). \quad (3)$$

The four states we consider are $|+, + \rangle, |-, + \rangle, |+, - \rangle$ and $|-, - \rangle$, where the first index specifies the spin projection, while the second one is the orbital projection. It's then obvious that the spin and orbital operators are expressed in terms of these four-component fermions as:

$$\begin{aligned} S_i^+ &= C_{i,1}^\dagger C_{i,2} + C_{i,3}^\dagger C_{i,4}, \\ S_i^- &= C_{i,2}^\dagger C_{i,1} + C_{i,4}^\dagger C_{i,3}, \\ S_i^z &= \frac{1}{2}(C_{i,1}^\dagger C_{i,1} - C_{i,2}^\dagger C_{i,2} + C_{i,3}^\dagger C_{i,3} - C_{i,4}^\dagger C_{i,4}); \end{aligned} \quad (4)$$

$$\begin{aligned} T_i^+ &= C_{i,1}^\dagger C_{i,3} + C_{i,2}^\dagger C_{i,4}, \\ T_i^- &= C_{i,3}^\dagger C_{i,1} + C_{i,4}^\dagger C_{i,2}, \\ T_i^z &= \frac{1}{2}(C_{i,1}^\dagger C_{i,1} + C_{i,2}^\dagger C_{i,2} - C_{i,3}^\dagger C_{i,3} - C_{i,4}^\dagger C_{i,4}), \end{aligned} \quad (5)$$

from which the following commutation relations can be proved

$$\begin{aligned} [S_i^+, S_j^-] &= 2S_i^z \delta_{i,j}, & [S_i^z, S_j^\pm] &= \pm S_i^\pm \delta_{i,j}, \\ [T_i^+, T_j^-] &= 2T_i^z \delta_{i,j}, & [T_i^z, T_j^\pm] &= \pm T_i^\pm \delta_{i,j}, \\ [S_i^\alpha, T_j^\beta] &= 0, & \alpha, \beta &= x, y, z. \end{aligned} \quad (6)$$

It is thus demonstrated that the spin and orbital operators are two independent degrees of freedom and both of them obey their respective SU(2) Lie algebra. By imposing a local constraint $\sum_{\mu} C_{i,\mu}^{\dagger} C_{i,\mu} = 1$, we can further prove that constraints $\mathbf{S}_i^2 = \mathbf{T}_i^2 = 3/4$ are satisfied, corresponding to the spin-1/2 system with two-fold orbital degeneracy. Under the new representation, the model Hamiltonian is expressed as a quadratic form in terms of two composite operators

$$H = -J_c \sum_i : A_i^{\dagger} A_i : - J_s \sum_i B_i^{\dagger} B_i, \quad (7)$$

with

$$\begin{aligned} A_i &= \sum_{\mu} C_{i+1,\mu}^{\dagger} C_{i,\mu}, \\ B_i &= [(C_{i+1,4} C_{i,1} + C_{i+1,1} C_{i,4}) \\ &\quad - (C_{i+1,3} C_{i,2} + C_{i+1,2} C_{i,3})], \end{aligned} \quad (8)$$

where A_i describes a nearest neighbor VB hopping parameter, while B_i represents a nearest neighbor VB pairing parameter. The normal ordering has been chosen in the first term.

To develop a MF theory, the nearest neighbor VB order parameters are defined by $\Delta_c(i) = \langle A_i \rangle$ and $\Delta_s(i) = -\langle B_i \rangle$. The model Hamiltonian is then decomposed into

$$\begin{aligned} \mathcal{H} &= -J_c \sum_{i,\mu} [\Delta_c(i) C_{i,\mu}^{\dagger} C_{i+1,\mu} + H.c.] + \lambda \sum_{i,\mu} C_{i,\mu}^{\dagger} C_{i,\mu} \\ &\quad + J_s \sum_i [\Delta_s(i) (C_{i,1}^{\dagger} C_{i+1,4}^{\dagger} + C_{i,4}^{\dagger} C_{i+1,1}^{\dagger}) \\ &\quad - \Delta_s(i) (C_{i,2}^{\dagger} C_{i+1,3}^{\dagger} + C_{i,3}^{\dagger} C_{i+1,2}^{\dagger}) + H.c.] \\ &\quad - \lambda N + N [J_c |\Delta_c(i)|^2 + J_s |\Delta_s(i)|^2], \end{aligned} \quad (9)$$

where a local chemical potential is first introduced to impose the local constraint and then it is replaced by a global value λ keeping the translational symmetry. When the spatial uniformity of VB parameters are also assumed, in terms of a generalized Nambu spinor,

$$\Psi_k^{\dagger} = (C_{k,1}^{\dagger}, C_{k,2}^{\dagger}, C_{k,3}^{\dagger}, C_{k,4}^{\dagger}, C_{-k,1}, C_{-k,2}, C_{-k,3}, C_{-k,4})$$

the MF model Hamiltonian can be rewritten in a compact form

$$\mathcal{H} = \frac{1}{2} \sum_k \Psi_k^{\dagger} \mathbf{H}_{mf}(k) \Psi_k + \lambda N + N (J_c \Delta_c^2 + J_s \Delta_s^2),$$

where $\mathbf{H}_{mf}(k) = [\lambda - \Delta_c(k)] \mathbf{\Omega}_1 - \Delta_s(k) \mathbf{\Omega}_2$, $\Delta_c(k) = 2J_c \Delta_c \cos k$, $\Delta_s(k) = (2J_s \Delta_s \sin k)$ with $\mathbf{\Omega}_1 = \sigma_z \otimes \sigma_0 \otimes \sigma_0$ and $\mathbf{\Omega}_2 = \sigma_x \otimes \sigma_y \otimes \sigma_y$. The corresponding Lagrangian is given by

$$L_{mf} = \frac{1}{2} \sum_k \Psi_k^{\dagger}(i\omega_n) [i\omega_n - \mathbf{H}_{mf}(k)] \Psi_k(i\omega_n) + \dots$$

the Matsubara Green's function matrix is thus derived as

$$\mathbf{G}(k, i\omega_n) = \frac{i\omega_n + [\lambda - \Delta_c(k)]\Omega_1 - \Delta_s(k)\Omega_2}{(i\omega_n)^2 - [\lambda - \Delta_c(k)]^2 - \Delta_s^2(k)}. \quad (10)$$

Then the fermionic excitation spectra with fourfold degeneracy are yielded

$$\epsilon_k = \pm \sqrt{(\lambda - 2J_c\Delta_c \cos k)^2 + (2J_s\Delta_s \sin k)^2}. \quad (11)$$

In the excitation spectra (with plus sign), the local energy minima appear at the specific momentum – the so-called Fermi momentum k_F , where an energy gap opens up when $\Delta_s \neq 0$.

Now consider the static properties at zero temperature. By filling in all states with negative energies, the ground state energy per site is evaluated as

$$\begin{aligned} \varepsilon_g = & - \int_{-\pi}^{\pi} \frac{dk}{\pi} \sqrt{(\lambda - 2J_c\Delta_c \cos k)^2 + (2J_s\Delta_s \sin k)^2} \\ & + \lambda + (J_c\Delta_c^2 + J_s\Delta_s^2). \end{aligned} \quad (12)$$

By minimizing the ground state energy with respect to parameters Δ_c , Δ_s , and λ , the saddle point equations are derived as:

$$\begin{aligned} \int_{-\pi}^{\pi} \frac{dk}{\pi} \frac{-(\lambda - 2J_c\Delta_c \cos k) \cos k}{\sqrt{(\lambda - 2J_c\Delta_c \cos k)^2 + (2J_s\Delta_s \sin k)^2}} &= \Delta_c, \\ \int_{-\pi}^{\pi} \frac{dk}{\pi} \frac{2J_s \sin^2 k}{\sqrt{(\lambda - 2J_c\Delta_c \cos k)^2 + (2J_s\Delta_s \sin k)^2}} &= 1, \\ \int_{-\pi}^{\pi} \frac{dk}{\pi} \frac{(\lambda - 2J_c\Delta_c \cos k)}{\sqrt{(\lambda - 2J_c\Delta_c \cos k)^2 + (2J_s\Delta_s \sin k)^2}} &= 1. \end{aligned} \quad (13)$$

In particular, when $V/J = 4$, the self-consistent equations are easily solved, and we obtain $\lambda = 4J/\pi$, $\Delta_c = 2\sqrt{2}/\pi$, and $\Delta_s = 0$. There are four degenerate gapless fermionic energy bands, different from the three bosonic elementary excitations obtained from the Bethe ansatz method [16]. However, as will be shown later, there are only three gapless collective (bosonic) excitations, so the physical conclusions are correct. The reason why four, instead of three, gapless modes show up in the fermion representation is similar to the weak coupling limit of the effective bosonization approach [6]. In that approach the charge excitation becomes gapped in the strong coupling limit due to an unklapp term, whereas the other three branches remain degenerate and gapless with marginally irrelevant interactions [6]. Away from the SU(4) symmetric point $V/J < 4$, numerical calculations can be performed and solutions to these self-consistent equations are derived: λ and Δ_c steadily decrease as the coupling parameter V/J is reduced, while Δ_s gradually increases at the same time.

The ground state energy per site is plotted as a function of the coupling parameter V/J in Fig.1. In order to compare two limiting cases, the corresponding ground state energies for $\Delta_c \neq 0$, $\Delta_s = 0$ and $\Delta_c = 0$, $\Delta_s \neq 0$ are also plotted in the same figure as well. It has been found that the gapped phase ($\Delta_c \neq 0$ and $\Delta_s \neq 0$) is smoothly connected with the strong coupling SU(4) symmetric gapless phase ($\Delta_c \neq 0$, $\Delta_s = 0$), and represents the possible lowest ground energy state in the parameter range of $0.462 < V/J \leq 4$. Our strong coupling MF theory is probably limited to this regime.

In Fig.2 the fermionic quasiparticle spectra with both positive and negative energies are plotted in the range $[-\pi/2, \pi/2]$ for different couplings $V/J = 3.85, 2.00, 1.265, 0.8$. In particular, at a special value of $(V/J)_c \sim 1.265$, both spectra in the range $[-k_F, k_F]$ become completely flat. Furthermore, for $V/J > (V/J)_c$, the minimum point of the spectra appears at a finite Fermi momentum $\pm k_F$, while for $V/J < (V/J)_c$ the minimum point of the spectra is shifted to zero. The special value of $(V/J)_c$ is very close to the exactly soluble point of $V/J = 4/3$ of the model Hamiltonian [18].

The Fermi momentum in the excitation spectrum mentioned above is given by

$$k_F = \cos^{-1} \left[\frac{\lambda(2J_c\Delta_c)}{(2J_c\Delta_c)^2 - (2J_s\Delta_s)^2} \right], \quad (14)$$

which is also calculated as a function of V/J and plotted in Fig.3a. It has been found that k_F is almost fixed at $\pi/4$ over a large range of $2 \leq V/J \leq 4$, and then quickly decreases to zero near the point of $V/J \sim 1.18$. The energy gap opens up at momentum k_F and is evaluated as

$$\Delta_{gap} = \sqrt{(2J_s\Delta_s)^2 + \frac{\lambda^2(2J_s\Delta_s)^2}{|(2J_c\Delta_c)^2 - (2J_s\Delta_s)^2|}}, \quad (15)$$

which is presented in Fig. 3b. In the range of $3 < V/J < 4$, the energy gap is extremely small. This agrees with the recent density matrix renormalization group calculations showing exponentially slow gap opening [7], in contrast to the earlier results [3]. Only when $V/J < 3$, the energy gap starts to grow slowly up to a maximum near the critical value $(V/J)_c \sim 1.265$, and then decreases to a very small value near $V/J \sim 0.462$. The position of the maximum energy gap roughly corresponds to the condition of the dispersionless quasiparticle excitations, which is consistent with the analysis at the exactly soluble point [18].

In the present strong coupling MF theory, the spin-spin and orbital-orbital density correlation functions can simply be evaluated as well. The spin and orbital density operators Eq. (4) are re-expressed in terms of the generalized Nambu spinor

$$\begin{aligned} S_i^\alpha &= \frac{1}{4} \Psi_i^\dagger \Omega_S^\alpha \Psi_i, \quad T_i^\alpha = \frac{1}{4} \Psi_i^\dagger \Omega_T^\alpha \Psi_i, \\ \Omega_S^x &= \sigma_z \otimes \sigma_0 \otimes \sigma_x, \quad \Omega_S^y = \sigma_0 \otimes \sigma_0 \otimes \sigma_y, \\ \Omega_S^z &= \sigma_z \otimes \sigma_0 \otimes \sigma_z, \quad \Omega_T^x = \sigma_z \otimes \sigma_x \otimes \sigma_0, \\ \Omega_T^y &= \sigma_0 \otimes \sigma_y \otimes \sigma_0, \quad \Omega_T^z = \sigma_z \otimes \sigma_z \otimes \sigma_0. \end{aligned}$$

Then the spin and orbital density-density correlation functions are given by

$$\chi_X^\alpha(q, i\omega_m) = -\frac{1}{16\beta} \sum_{\omega_n} \int \frac{dk}{2\pi} \text{Tr} [\Omega_X^\alpha \mathbf{G}(k, i\omega_n) \Omega_X^\alpha \mathbf{G}(k+q, i\omega_m + i\omega_n)], \quad (16)$$

where $\Omega_X^\alpha = \Omega_S^\alpha$ for the spin and $\Omega_X^\alpha = \Omega_T^\alpha$ for the orbital. By inserting the Matsubara Green function, it is straightforward to prove the following relation,

$$\chi_S^\alpha(q, i\omega_m) = \chi_T^\alpha(q, i\omega_m) \equiv \chi(q, i\omega_m), \quad (17)$$

independent of the indices $\alpha = x, y, z$. This shows that away from the SU(4) symmetry point, the spin and orbital rotational symmetry of SU(2)⊗SU(2) with an additional Z₂ symmetry in exchange between \mathbf{S}_i and \mathbf{T}_i is satisfied in the present strong coupling MF state. The resulting expression of $\chi(q, i\omega_m)$ is given by

$$\chi(q, i\omega_m) = -\frac{1}{2\beta} \sum_{\omega_n} \int \frac{dk}{2\pi} \frac{i\omega_n(i\omega_m + i\omega_n) + (\lambda - \Delta_c(k))(\lambda - \Delta_c(k+q)) + \Delta_s(k)\Delta_s(k+q)}{[(i\omega_n)^2 - \epsilon_k^2][(i\omega_m + i\omega_n)^2 - \epsilon_{k+q}^2]}. \quad (18)$$

However, in the SU(4) spin-fermion representation, nine spin-orbital tensor operators associated with nonlinear collective excitation of both spin and orbital degrees of freedom, can be defined by $L_i^{\alpha,\beta} = 2S_i^\alpha T_i^\beta$, which can also be expressed in terms of the generalized Nambu spinor as

$$\begin{aligned} L_i^{\alpha,\beta} &= \frac{1}{4} \Psi_i^\dagger \Omega_L^{\alpha,\beta} \Psi_i, \\ \Omega_L^{xx} &= \sigma_z \otimes \sigma_x \otimes \sigma_x, \quad \Omega_L^{xy} = \sigma_0 \otimes \sigma_y \otimes \sigma_x, \\ \Omega_L^{xz} &= \sigma_z \otimes \sigma_z \otimes \sigma_x, \quad \Omega_L^{yx} = \sigma_0 \otimes \sigma_x \otimes \sigma_y, \\ \Omega_L^{yy} &= \sigma_z \otimes \sigma_y \otimes \sigma_y, \quad \Omega_L^{yz} = \sigma_0 \otimes \sigma_z \otimes \sigma_y, \\ \Omega_L^{zx} &= \sigma_z \otimes \sigma_x \otimes \sigma_z, \quad \Omega_L^{zy} = \sigma_0 \otimes \sigma_y \otimes \sigma_z, \\ \Omega_L^{zz} &= \sigma_z \otimes \sigma_z \otimes \sigma_z. \end{aligned} \quad (19)$$

Then it can be proved that the corresponding nine correlation functions $\langle T_\tau L_i^{\alpha,\beta}(\tau) L_j^{\alpha,\beta}(\tau') \rangle$ are the same, and equal to

$$\chi_L(q, i\omega_m) = -\frac{1}{2\beta} \sum_{\omega_n} \int \frac{dk}{2\pi} \frac{i\omega_n(i\omega_m + i\omega_n) + (\lambda - \Delta_c(k))(\lambda - \Delta_c(k+q)) - \Delta_s(k)\Delta_s(k+q)}{[(i\omega_n)^2 - \epsilon_k^2][(i\omega_m + i\omega_n)^2 - \epsilon_{k+q}^2]}. \quad (20)$$

Compared to the spin and orbital density correlation functions, there is only a sign difference in front of $\Delta_s(k)\Delta_s(k+q)$. In the conventional response function theory, the correlation spectrum $\chi_L(q, i\omega_m)$ represents a *nonlinear* collective excitations of both spins and orbitals. When $V/J = 4$, it is found that $\Delta_s = 0$, and then we have $\chi_L^{\alpha\beta}(q, i\omega_m) = \chi_S^\alpha(q, i\omega_m) = \chi_T^\alpha(q, i\omega_m)$, independent of their component indices of spin and orbital operators, which implies that the SU(4) symmetry is recovered.

After summation over the Matsubara frequency and analytical continuation, we find that in both dynamic susceptibilities $\chi(q, \omega)$ and $\chi_L(q, \omega)$, an energy gap exists at $\omega = 2\Delta_{gap}$ in the large parameter range of $0.462 < V/J < 4$. As far as the relevant experiments [1,2] are concerned, however, the most important physical quantities measured are the corresponding static susceptibilities. In the zero frequency limit, the static susceptibilities $\chi(q)$ and $\chi_L(q)$ are deduced to respectively

$$\begin{pmatrix} \chi(q) \\ \chi_L(q) \end{pmatrix} = \int \frac{dk}{8\pi} \left\{ \frac{[n_F(\epsilon_k) - n_F(\epsilon_{k+q})]}{\epsilon_{k+q} - \epsilon_k} \left[1 + \frac{(\lambda - \Delta_c(k))(\lambda - \Delta_c(k+q)) \pm \Delta_s(k)\Delta_s(k+q)}{\epsilon_k \epsilon_{k+q}} \right] \right. \\ \left. + \frac{[1 - n_F(\epsilon_{k+q}) - n_F(\epsilon_k)]}{\epsilon_{k+q} + \epsilon_k} \left[1 - \frac{(\lambda - \Delta_c(k))(\lambda - \Delta_c(k+q)) \pm \Delta_s(k)\Delta_s(k+q)}{\epsilon_k \epsilon_{k+q}} \right] \right\}.$$

We present the static spin and orbital susceptibility at zero temperature in Fig.4 and the static spin-orbital tensor susceptibility at zero temperature in Fig.5 for different coupling parameters $V/J = 2.72, 2.00, 1.265, 0.80,$ and 0.50 .

At $V/J = 2.72$, since the energy gap in the elementary excitations is negligible, both static susceptibilities $\chi(q)$ and $\chi_L(q)$ have sharp peaks at $q = \pm\pi/2$, corresponding to a commensurate spin- and orbital-density wave of period four. The period four arises because the spin and orbital chain are in their $SU(4)$ fundamental representation and by "quadruplicity" one needs four sites to form a singlet. Moreover, as the momentum goes to zero, $\chi(q)$ approaches to zero, while $\chi_L(q)$ to a constant.

As V/J decreases further, a finite gap opens up, and the sharp peaks in both $\chi(q)$ and $\chi_L(q)$ spectra at $q = \pm\pi/2$ are strongly suppressed and broadened. Meanwhile, the peak positions are slightly shifted to lower momenta, indicating the possible presence of incommensurate density waves in the gapped phase. The spectral weights of the coherent quasiparticle peaks are gradually transferred to the incoherent excitations at $q = \pm\pi$ for $\chi(q)$ and at $q = 0$ for $\chi_L(q)$. Thus, the static spin and orbital susceptibilities around $q = \pm\pi$ are enhanced, exhibiting a crossover from coherent to incoherent magnetic excitations. Some of these features have been speculated by an effective low-energy bosonization theory [6,14]. From our MF theory, the crossover is estimated to occur around the critical coupling $V/J = 1.265$. It seems to us that the present symmetric state is a good approximation of the genuine ground state to describe this crossover. Moreover, the spectrum of $\chi_L(q)$ in Fig.5 displays a further clear evidence of the crossover of the magnetic excitations from the strong to weak coupling limits of the system. In particular, when V/J becomes smaller and smaller, a new peak structure clearly emerges at zero momentum. All these features of $\chi_L(q)$ are new results obtained from the present non-perturbative theory.

Finally, several remarks and comments are in order. i) The fermionic MF theory developed in this paper mainly focuses on the energy gap formation of the spin-orbital coupled model, in particular, on the crossover of coherent-incoherent magnetic excitations in the gapped phase. ii) All the obtained results on the gapped phase are mostly consistent with the latest density matrix renormalization group calculation [7] and the effective bosonization theory [6]. One of the important results is that the energy gap opens up extremely slowly away from the $SU(4)$ symmetric point, indicating that the phase transition from gapless to gapped phases may be of Kosterlitz-Thouless type. The gapped regime with coherent magnetic excitations shares some similarities with the Haldane gapped phase of the quantum antiferromagnetic spin-ladder model with a four-spin interaction [14]. So it is not clear whether the Lieb-Schultz-Mattis theorem is valid in the present spin-orbital coupled system or not. iii) The gapless phase at the $SU(4)$ point is only characterized by a Fermi liquid behavior in the present MF theory approximately, different from the Luttinger liquid behavior derived from the Bethe ansatz and effective field theories [16,17,6]. However, as far as the spin, orbital, and spin-orbital tensor collective excitations are concerned, all these physical results of the spin-orbital system — the correlation spectra are in good agreement with the exact solution.

In conclusion, we have applied an $SU(4)$ constraint fermion representation to a one-dimensional symmetrically coupled spin-orbital model, a spin-orbital gapped phase is generated away from the strong coupling $SU(4)$ symmetric point by a relevant spin-orbital pairing interaction. The energy gap of the elementary spin and orbital excitations grows extremely

slowly up to a maximum value and then decreases. The spin, orbital, and spin-orbital tensor static susceptibilities are also calculated at zero temperature, displaying a crossover from coherent to incoherent magnetic excitations as the spin-orbital coupling decreasing away from the $SU(4)$ symmetry point. It is interesting to note that the present mean field theory provides a rather good description of the underlying physics over a large crossover region between the two critical points. It's likely that the $SU(4)$ constraint fermion representation is appropriate for this system.

We would like to thank Prof. Z. B. Su and X. Q. Wang for useful discussions, while L. Yu would like to thank A. Nersesyan for very helpful comments. This work is supported by NSF-China (Grant No. 10074036 and 10125418) and the Special Fund for Major State Basic Research Projects of China (G2000067107).

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Figure Captions

Fig. 1. The ground state energy per site as a function of the coupling parameter V/J . For comparison, the corresponding ground state energies for $\Delta_c \neq 0, \Delta_s = 0$ and $\Delta_c = 0, \Delta_s \neq 0$ are also plotted by the dashed and dash-dotted lines, respectively.

Fig. 2. The fermionic energy spectra are plotted in the range $[-\pi/2, +\pi/2]$ for the coupling values: a) $V/J = 3.85, 2.00$ and b) $V/J = 1.265, 0.80$.

Fig. 3. The Fermi momentum k_F and the corresponding quasiparticle gap as functions of coupling parameter V/J .

Fig. 4. The static spin and orbital susceptibilities at zero temperature for different coupling values: a) $V/J = 2.72, 2.00$ and b) $V/J = 1.265, 0.80, \text{ and } 0.50$.

Fig. 5. The static susceptibility of the spin-orbital tensor at zero temperature for different coupling values: a) $V/J = 2.72, 2.00$ and b) $V/J = 1.265, 0.80, \text{ and } 0.50$.

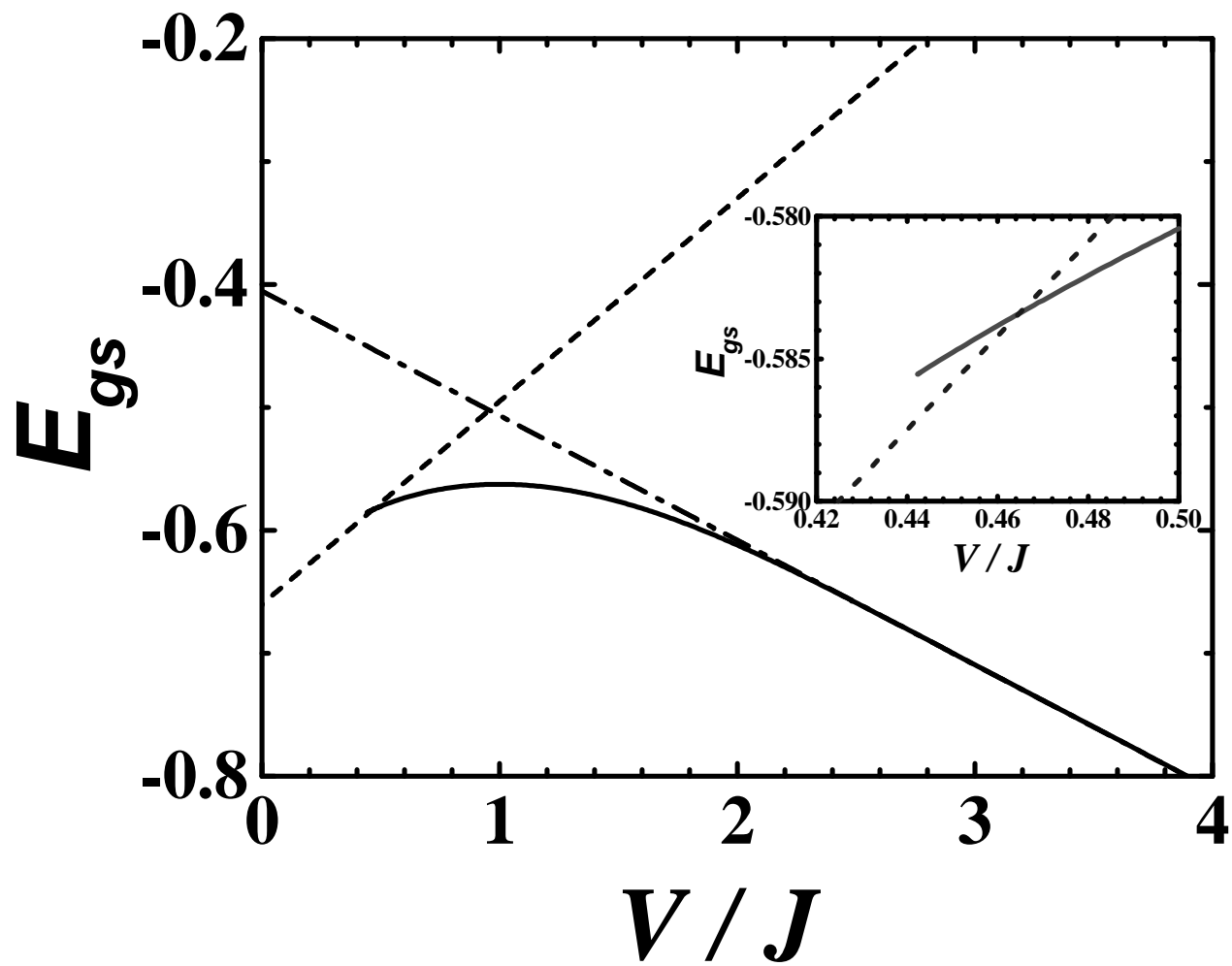


Figure 1

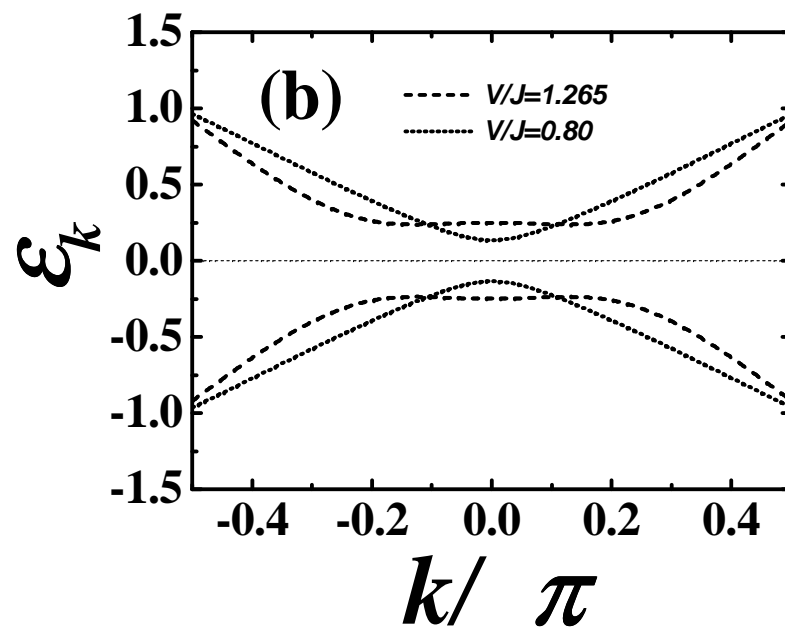
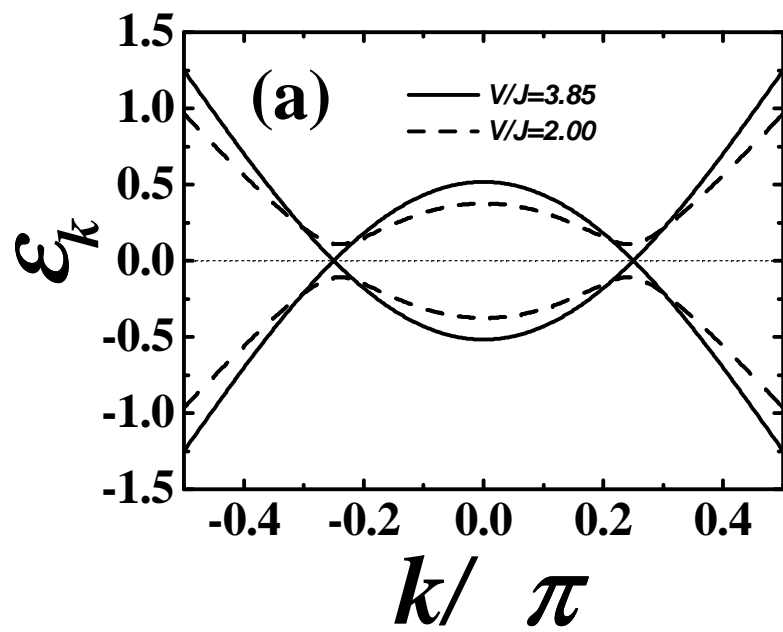


Figure2

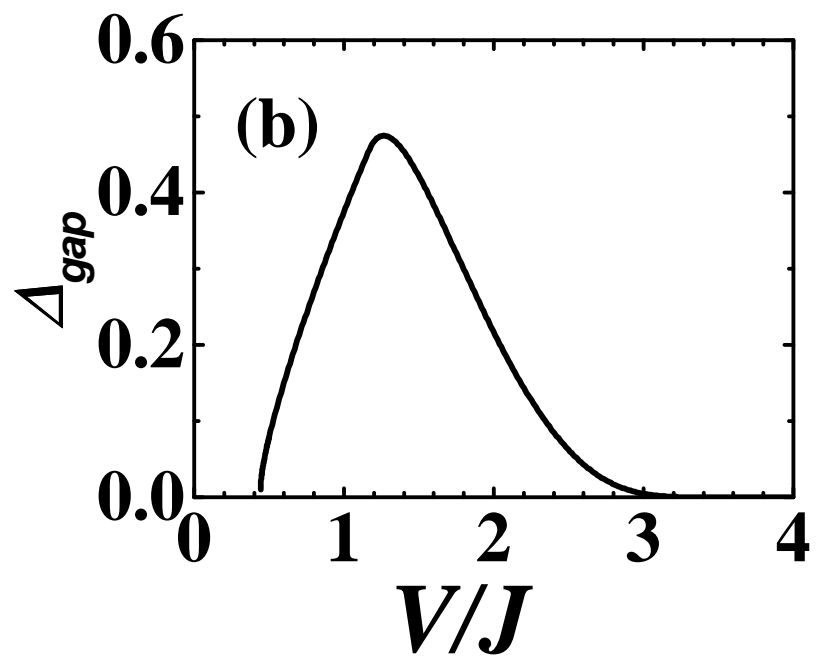
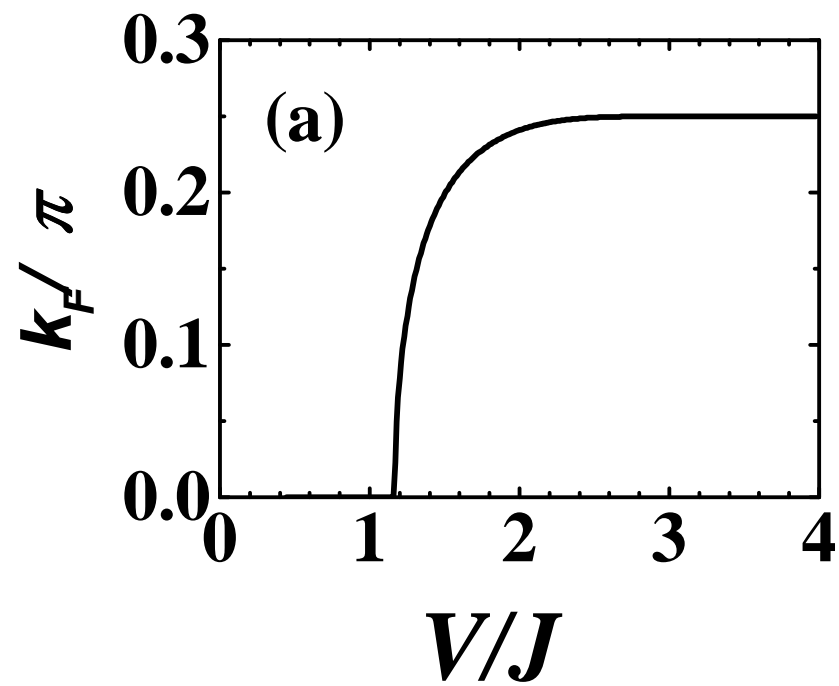


Figure3

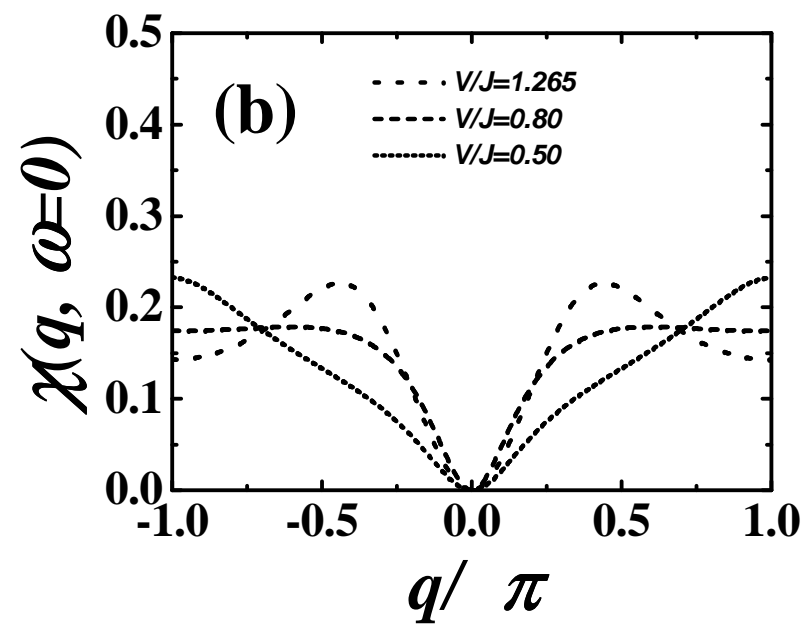
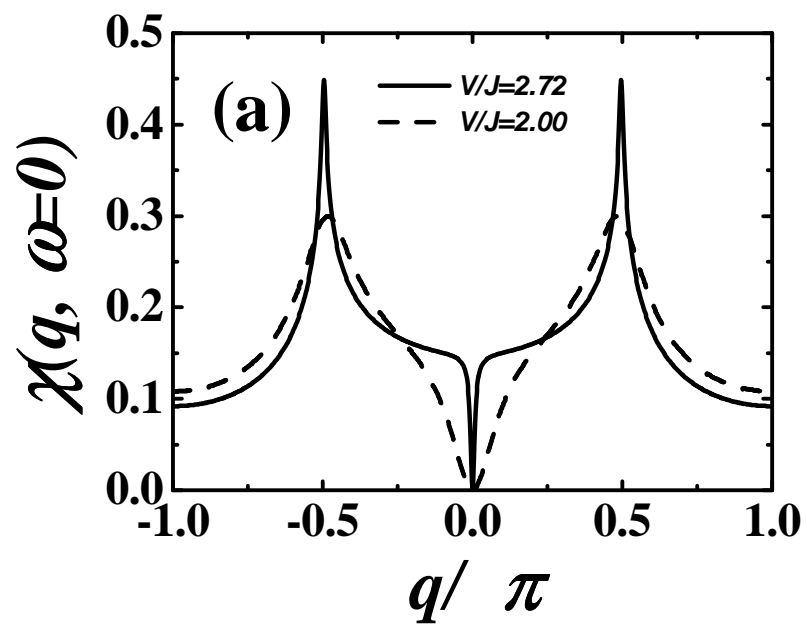


Figure4

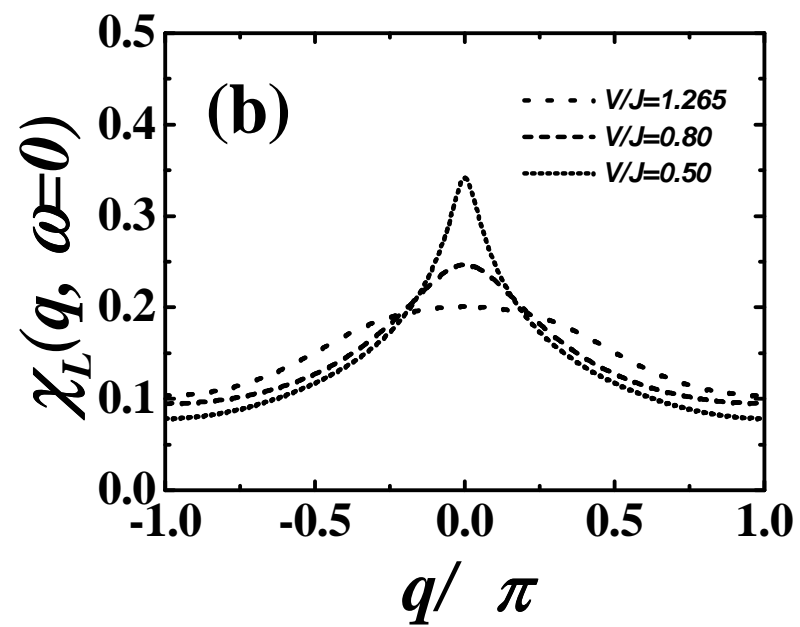
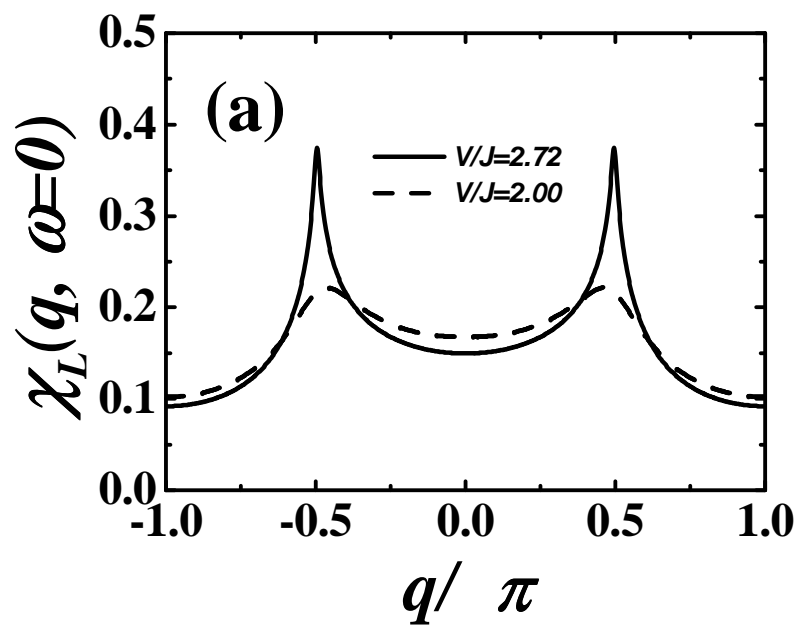


Figure5