Exact solution for spin-orbiton excitations on a ferromagnetically ordered finite chain

S. Cojocaru* and A. Ceulemans

Division of Quantum Chemistry, University of Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium (Received 22 December 2002; published 13 June 2003)

The finite chain of singly occupied twofold degenerate orbital sites with Hund's rule coupling is considered. The equation of motion for the combined spin and orbital excitation is solved exactly. The structure and stability of bound versus scattered states are examined and the critical momenta for state crossing are determined. The solutions are also extended to the thermodynamic limit of an infinite chain and compared to the existing spin-orbiton descriptions [Van den Brink *et al.*, Phys. Rev. B **58**, 10 276 (1998)]. The possibility to probe orbiton dynamics via spin excitations is discussed.

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I. INTRODUCTION

Orbital degrees of freedom are especially important for the systems containing transition metal ions with degenerate or pseudodegenerate strongly correlated energy levels such as cuprates, manganates, and vanadates. Besides of the interest related to the emerging new materials and their applications, these systems have attracted a large interest for their fundamental properties. Ordering and excitations of charge, spin, orbital, and other degrees of freedom in such systems are deeply interconnected, giving rise to a variety of new properties (see Ref. 1 for a review). A recent example is the experimental observation of the orbiton, a fundamental excitation in a solid with long-range ordering of electron orbitals, LaMnO₃.² The low-energy excitations can be described by means of effective models after projecting on the subspace of a relevant energy scale; for example, see Ref. 3. Generally, the coupling constants in such models are anisotropic, and antiferromagnetic ordering of one subsystem favors ferromagnetic ordering in the other one. However, there can exist situations when both subsystems order ferromagnetically. These can be associated with phase-separated or stripe phases observed at certain doping in manganites with colossal magnetoresistance such as $La_{1-x}Ca_xMnO_3$ or in transition-metal oxides such as NaNiO₂ with a layered frustrated lattice. A completely ferromagnetically coupled system was considered in Ref. 4, where a new type of composite, spin and orbital, bound excitation was described in the thermodynamic limit on one- and two-dimensional lattices. Bound excitations, being the lowest in energy, can be very important for the low-temperature response of the system, for the formation of inhomogeneous phases and others. In the present paper we describe an exact solution of this model for a finite chain. It allows us to obtain a deeper insight into the nature of the spin-orbiton excitation. It turns out that to understand the specific features of the bound excitation it is important to analyze the spectra of the scattering states, which are difficult to observe within the thermodynamic limit treatment itself.

II. THE EQUATION OF MOTION

We consider the following Hamiltonian describing the low-energy spin and orbital excitations of electrons in doubly degenerate orbital states:

$$H = -\sum_{i=0}^{N-1} [J_{S} \mathbf{S}_{i} \cdot \mathbf{S}_{i+1} + J_{T} \mathbf{T}_{i} \cdot \mathbf{T}_{i+1} + 4J_{ST} (\mathbf{S}_{i} \cdot \mathbf{S}_{i+1}) \times (\mathbf{T}_{i} \cdot \mathbf{T}_{i+1})], \qquad (1)$$

where both S_i and T_i are spin-1/2 angular momentum operators describing spin and orbital degrees of freedom, respectively, on a chain of N sites with periodic boundary conditions and the subscripts of the constants J refer to respective couplings. Qualitative arguments and the energy spectrum were given to prove the existence of the combined bound state for arbitrary interaction strength⁴ in analogy with the two-magnon excitation in a simple ferromagnet.⁵ This bound state was found to be the lowest-energy elementary excitation of the system. We show that in the thermodynamic limit there exist two combined bound-state modes (ST) that differ by symmetry of the wave function but have the same dispersion. However, these are not the lowest-energy excitations: for any choice of parameters corresponding to the ferromagnetic ground state either the two-magnon (SS) or the twoorbiton (TT) modes, or both of them have a lower excitation energy at any momenta. Moreover, if magnons and orbitons have a different stiffness, i.e., $x \equiv J_S - J_T \neq 0$, there exists a critical value of x beyond which the ST bound state disappears at the edge of the Brillouin zone, $P = \pi$. For a finite lattice the instability of the ST excitation becomes even more dramatic. The spectrum splits into two branches and both bound states merge with the continuum of scattered states in finite areas close to the P=0 and $P=\pi$. This behavior is in contrast to the pure SS or TT excitations, where a stable bound state exists for arbitrary momenta.

The spin-orbiton excitation is defined in the usual way,

$$|\psi\rangle = \sum_{0 \le n_1, n_2 \le N-1} a_{ST}(n_1, n_2) S_{n_1}^- T_{n_2}^- |0\rangle,$$

where the ground state $|0\rangle$ is the fully aligned state of maximum *S* and *T*. By separating the total momentum *P* we introduce the amplitude of the relative distance $X = n_2 - n_1$ between spin and orbital flips,

$$a_{ST}(n_1, n_2) = \exp\left(iP\frac{n_1 + n_2}{2}\right)A(X),$$
 (2)

which is decomposed in the Fourier series

$$A(X) = \frac{1}{\sqrt{N}} \sum_{Q} \exp(iQX)B(Q).$$
(3)

From the periodic boundary conditions $a_{ST}(n_1, n_2) = a_{ST}(n_1+N, n_2+N)$ and $a_{ST}(n_1, n_2) = a_{ST}(n_1, n_2+N)$ one obtains the quantization of the total momentum $P = 2\pi k/N$, k = 0, 1, ..., N-1 and a relation satisfied by the amplitude of relative motion

$$A(X) = \exp(i\pi k)A(X+N).$$
(4)

The latter allows us to classify the states into symmetric (*s*) and antisymmetric (*a*) categories, depending on even or odd values of *k*. As a consequence of this relation one obtains two sequences of values for *Q* in the Fourier expansion (3): $Q^s = 2\pi m/N$ or $Q^a = 2\pi (m + \frac{1}{2})/N$, m = 0, 1, ..., N-1. By taking the Fourier transform of the equation of motion we obtain

$$B(Q)\left\{E - (J_{S}+1)\left[1 - \cos\left(\frac{P}{2} - Q\right)\right]\right\}$$
$$- (J_{T}+1)\left[1 - \cos\left(\frac{P}{2} + Q\right)\right]\right\}$$
$$= -4\left[\cos\left(\frac{P}{2}\right) - \cos(Q)\right]\frac{1}{N}\sum_{Q'}B(Q')$$
$$\times \left[\cos\left(\frac{P}{2}\right) - \cosQ'\right], \tag{5}$$

where the excitation energy *E* and the coupling constants are scaled with the spin-orbital coupling constant $E \rightarrow E/J_{ST}$, $J_S \rightarrow J_S/J_{ST}$, $J_T \rightarrow J_T/J_{ST}$. For a fixed momentum *P* the amplitude is

$$B(Q) = \frac{C\cos\delta}{\cos(P/2)(2+2J_T+x)} \frac{\cos(P/2) - \cos Q}{\cosh v - \cos(Q-\delta)}, \quad (6)$$

where we have introduced two phase variables:

$$\delta = \arctan\left[\tan\left(\frac{P}{2}\right)\frac{J_S - J_T}{2 + J_S + J_T}\right],\tag{7}$$
$$v = \arccos\left[\frac{\cos(\delta)}{\cos(P/2)}\left(1 - \frac{E}{2 + J_S + J_T}\right)\right].$$

Iterating the definition of the constant $C = (4/N)\Sigma_Q B(Q)[\cos(P/2) - \cos Q]$ leads to the eigenenergy equation

$$1 = \frac{4\cos(\delta)}{N(2+J_S+J_T)\cos(P/2)} \sum_{m=0}^{N-1} \frac{[\cos(P/2) - \cos Q_m]^2}{\cosh v - \cos(Q_m - \delta)}.$$
(8)

The integral form of this equation for $N \rightarrow \infty$ coincides with the result in Ref. 4 up to a factor of 2 used to scale the coupling constants. The meaning of introducing the variables in Eq. (7) becomes now clear: bound states, if any, correspond to a real-valued positive solution for v in Eq. (8) while scattered states, which are related to the singularities of the denominator, correspond to purely imaginary values of v. The threshold value v=0 establishes a separation line between the two types of solutions:

$$E_{c} = 2 + J_{S} + J_{T} - \sqrt{4 \cos^{2} \left(\frac{P}{2}\right) (1 + J_{T}) (1 + J_{S}) + (J_{S} - J_{T})^{2}}.$$
 (9)

The phase δ quantifies the difference of dynamic properties of magnon and orbiton excitations throughout the Brillouin zone. The values of $\delta \in [0, \pi/2]$ and increase from the center towards the edge.

III. EXACT SOLUTION FOR THE FINITE CHAIN

To solve Eq. (5) we use the following general expressions for finite sums (details of derivation to be given elsewhere):

$$\frac{\sinh v}{N} \sum_{m=0}^{N-1} \frac{\sin[(\theta/N + 2\pi m/N)X]}{\cosh v - \cos(\theta/N + \delta + 2\pi m/N)} = \frac{1}{2i} \frac{\sinh[(v+i\delta)(N/2 - X) + i\theta/2]}{\sinh[(v+i\delta)N/2 + i\theta/2]} - \frac{1}{2i} \frac{\sinh[(v-i\delta)(N/2 - X) - i\theta/2]}{\sinh[(v-i\delta)N/2 - i\theta/2]}$$

$$\frac{\sinh v}{N} \sum_{m=0}^{N-1} \frac{\cos[(\theta/N + 2\pi m/N)X]}{\cosh v - \cos(\theta/N + \delta + 2\pi m/N)} = \frac{\cosh[(v+i\delta)(N/2 - X) + i\theta/2]}{2\sinh[(v+i\delta)N/2 + i\theta/2]} + \frac{\cosh[(v-i\delta)(N/2 - X) - i\theta/2]}{2\sinh[(v-i\delta)N/2 - i\theta/2]}, \quad (10)$$

where the phase variables can take complex values and $X \in [0, N-1]$. Extension outside the physical interval is described by Eq. (4). For instance, one can check that with (10) Bethe's solution for a spin chain is recovered at once without making an ansatz. We note that for the considered system the solution of Bethe's problem describes either the two magnon or two orbiton excitation with renormalized exchange interactions: $J = J_S + J_{ST}$ and $J = J_T + J_{ST}$ respectively. The values of θ for the combined ST excitation are fixed by the condition $\theta = PN$ in (10). As a result we obtain the following equation for the eigenenergy, irrespective of the symmetry of the mode:

EXACT SOLUTION FOR SPIN-ORBITON EXCITATIONS

$$\frac{(J_{S}+J_{T}-2)\cos(P/2)\sinh(v)}{4\cos(\delta)} = \left[\cos\left(\frac{P}{2}\right) - e^{-v}\cos(\delta)\right] \left[\cos\left(\frac{P}{2}\right) - e^{-v}\cos(\delta) - \frac{\sinh(v)}{\cos(\delta)}\right] \\ + \frac{\exp[-N(v+i\delta)]}{\cos(PN) - \exp[-N(v+i\delta)]} \left[\cos\left(\frac{P}{2}\right) - \cosh[(v+i\delta)]\right]^{2} \\ + \frac{\exp[-N(v-i\delta)]}{\cos(PN) - \exp[-N(v-i\delta)]} \left[\cos\left(\frac{P}{2}\right) - \cosh[(v-i\delta)]\right]^{2}.$$
(11)

One can notice that the wildly oscillating terms containing (δN) in the last two lines of the equation are suppressed in thermodynamic limit, provided we are considering the bound states (real and positive values of v). In the simplest case, $J_S = J_T$, the behavior of the ST states is qualitatively similar to that of SS or TT excitations and coincides with Bethe's solution when $J_S = J_T = J_{ST}$. For instance, one finds that a stable bound state exists for an arbitrary magnitude of coupling constants at any finite momenta P. As in Bethe's solution, the antisymmetric bound state becomes unstable and decays into scattering states in the long-wavelength region of the Brillouin zone, which scales as $1/\sqrt{N}$. However, as soon as J_S and J_T become different, the distinctive features of the ST excitations begin to emerge. Both symmetric and antisymmetric bound states states become unstable at small momenta P, i.e., they cross the boundary of scattering states at some $P = P_c \ll 1$. Let us consider the symmetric excitation. Solving Eq. (11) for $v(P_c) = 0$ leads to

$$P_{c}^{4} = \frac{2}{N} (J_{S} + J_{T} - 2) \sin^{2} \left(\frac{J_{S} - J_{T}}{2 + J_{S} + J_{T}} \frac{P_{c}N}{4} \right) \\ \times \left(\frac{(2 + J_{S} + J_{T})^{2}}{(J_{S} + 1)(J_{T} + 1)} \right)^{2} + O\left(\frac{1}{N^{2}}\right).$$
(12)

Not only does the symmetric state become unstable, but also the region of instability has become discontinuous due to the oscillating term. But most unexpectedly, an instability appears for *short* wavelengths of the excitation, where one would normally expect the strongest binding and localization to take place. Indeed, for $|J_S - J_T| > 4J_{ST}$ a rather broad instability region is found from Eq. (11) close to the edge of the Brillouin zone $(\pi - P) \leq 1$:

$$P_{c} = \pi - \frac{\sqrt{J_{s} - J_{T} - 4}}{\sqrt{2N}} \frac{J_{s} - J_{T}}{J_{T} + 1} \left| \sin\left(\frac{P_{c}N}{4}\right) \right| + O\left(\frac{1}{N}\right), \tag{13}$$

where we have assumed that $J_S > J_T + 4$. If, alternatively, $J_T > J_S + 4$, then the indices *S* and *T* have to be interchanged. The same equations hold for the antisymmetric excitation by replacing sin with cos in Eqs. (12) and (13). We note that the long-wavelength critical point has moved to larger momenta $P_c \sim N^{-1/4}$ as compared to Bethe's spin chain $P_c \sim N^{-1/2}$, but most remarkably, the above equation contains multiple solutions for P_c for any finite $J_S \neq J_T$ because of the oscillating terms on the right-hand side (rhs) of the equations. This

means that in the critical regions of the Brillouin zone that scale as $N^{-1/4}$ close to P=0 and $N^{-1/2}$ close to $P=\pi$ one has to observe reentrant behavior of bound states. This behavior is a consequence of the radical change of the structure of scattering bands. Figure 1 illustrates the effect interaction has on the combined orbiton and magnon excitation bands at finite N. Due to the energy splittings at the crossings of noninteracting bands, the spectrum of the interacting bands acquires a layered structure with undulations within the layers. As a result, the lowest-energy dispersion curve is formed which corresponds to the "reentrant" bound state as is shown for the symmetric state by "zooming" into the area adjacent to the lower boundary of the scattered states $E_c(P)$ in Fig. 2. The difference between symmetric and antisymmetric states, which is very significant for purely spin excitations,⁷ is almost completely eliminated for the combined excitations, as can be seen by comparing Figs. 2 and 3. The period of the undulations of the ST bands is determined by δ and N. It decreases towards small momenta, where the bands become more similar to the monotonous SS bands (see, e.g., Ref. 6) if δ and N are small enough. At first sight, the short-wavelength behavior seems to be in contradiction with the physical arguments and calculations presented in Ref. 4. For instance, the short-wavelength instability of the bound state "survives" even in the thermodynamic limit. If the stiffness of orbitons is close to that of magnons one in-



FIG. 1. Dispersion curves of the combined antisymmetric spinorbiton excitation on a finite chain with N=8, $J_S=J_{ST}$, $J_T=2J_{ST}$ as defined by the solutions of Eq. (11). The dotted line corresponds to vanishing interaction of the pseudoparticles: v = 0 in Eq. (7). The continuous lines below (above) it correspond to bound (scattering) states, respectively.



FIG. 2. A few low-energy dispersion curves of the symmetric spin-orbiton excitation for N=62, $J_S=J_{ST}$, $J_T=6J_{ST}$. The energy of excitations is measured with respect to $E_c(P)$, which corresponds to v=0. The lowest curve illustrates the reentrant behavior of the bound state at long and short wavelengths of the excitation.

deed finds a stable bound state for the whole Brillouin zone in analogy with the two-magnon problem.⁴ However, at larger values the spin-orbiton bound state disappears at the edge of the Brillouin zone despite the Goldstone mode singularity, keeping its energy away from merging with continuum. Indeed, from the definitions (7) we have $\delta \rightarrow \pi/2$ and

$$\frac{\cos(P/2)}{\cos(\delta)}\Big|_{P\to\pi} = \frac{|J_T - J_S|}{2 + J_S + J_T}.$$

After substitution into Eq. (11) we obtain a simple relation:

$$\frac{|J_T - J_S|}{4} = e^{-v}.$$
 (14)

Since for a bound state v should be real and positive, this equation does not have solutions for $|J_S - J_T| > 4$. At the critical point the energy of the bound state reaches the lower boundary of the band of scattered states E_c , Eq. (9). Above this threshold Eq. (14) is no longer valid since v becomes purely imaginary and the description of the band of scattering states requires knowledge of finite size corrections contained in Eq. (11). Thus, for $|J_S - J_T| > 4$ the *ST* bound state exists at the intermediate momenta outside the critical regions described by Eqs. (12) and (13) and its energy almost coincides with the lower boundary of scattered states. These features demonstrate that the binding of mixed spin and orbiton excitations can actually be very weak even if the *ST* coupling is significant.

To understand the physical reason of these instabilities it is necessary to consider the behavior of the ST wave function on a finite chain. On one side, there is indeed an energy gain for the spin and orbital excitations to occur within the range of the ST coupling as explained in Ref. 4. Consequently, one expects that, just as in the spin-spin problem, a tightly bound spin-pseudospin soliton is formed which moves as a single entity over the lattice. The larger the number of excited spins, the larger the energy gain of having droplets of such excitations. This is essentially the mechanism of domain wall formation that clearly remains valid for the spin-orbiton system, provided $J_S = J_T$. One obtains a stable bound state for any momenta that behaves similarly to



FIG. 3. Dispersion curves of the antisymmetric spin-orbiton excitation for N=62, $J_S=J_{ST}$, $J_T=6J_{ST}$. The energy of excitations is measured with respect to $E_c(P)$ as in Fig. 2.

the one found by Bethe. However, the situation changes qualitatively when $|J_S - J_T| \neq 0$. This is reflected in the explicit form of the wave function following from the expressions (10):

$$A(X) \sim \exp\left[i\delta\left(\frac{N}{2} - X\right)\right] \left(\frac{\exp[v(N/2 - X)]}{\sinh\{N[v + i(P + \delta)]/2\}} + \frac{\exp[-v(N/2 - X)]}{\sinh\{N[v - i(P + \delta)]/2\}}\right).$$

First we note that a difference in the stiffness of the excitations means that the pseudo-particles move over the lattice with different velocity. From Eqs. (6)–(8) it also follows that δ is a measure of momentum exchanged between the two interacting pseudoparticles, and it becomes nonzero as soon as $|J_S - J_T| \neq 0$. This produces an oscillating factor $\exp(iX\delta)$ in the wave function. At short wavelengths we have δ $\sim \pi/2$ and the wave function changes sign on the distance of a lattice spacing. The dynamic potential represented by the variable v should be strong enough to make the binding possible. For the spin-spin problem, for instance, this is achieved due to the divergence of v at $P = \pi$, which leads to a strongly bound state of two spin deviations localized on strictly nearest-neighbor sites. But the dynamic potential itself depends on the difference $J_S - J_T$ and, as follows from Eq. (14), decreases very fast until it reaches zero at the critical value. Diminishing v leads to a more delocalized shape of the wave function, which allows the oscillating term to annihilate the effect of the attractive potential. This results in formation of a scattering or a resonance state, shown in Fig. 4. Away from the edge of the Brillouin zone the phase angle δ becomes smaller and the bound state is stabilized at intermediate momenta as illustrated by Figs. 3 and 4. However, the competition of binding, v, and unbinding, δ , tendencies determines the reentrant behavior in the critical regions, Eqs. (12) and (13). At longer wavelengths the bound state becomes unstable again due to the large extent of the wave function that has nodes $(\delta \neq 0)$ even for the symmetric state



FIG. 4. The resonance behavior of the relative amplitude of the symmetric state on a chain with N=20 and $|J_S-J_T|>4J_{ST}$ for a short-wavelength excitation, $P \leq \pi$.

as shown in Fig. 5. In a two-dimensional (2D) system the same physical mechanisms are operative, but the critical regions are governed by logarithmic terms in N, instead of power law dependencies.⁷ Therefore one has to expect that bound spin and orbital excitations would exist in a much more restricted region of the Brillouin zone at intermediate momenta. In a 3D system bound states are likely not to appear at all even in the thermodynamic limit.

Another distinctive property of the *ST* excitations is their stronger ability to destroy long range ordering in the system. Coupling of magnons and orbitons due to the biquadratic term in the Hamiltonian (1) acts to diminish the energy of the combined excitation. This leads to a stronger restriction such excitations set on the stability of the ground state, as compared to pure spin or orbital excitations. The restriction requires that excitation energy *E* be positive. Keeping only the main terms in Eq. (11) for the $P \ll 1$ expansion we find in the limit $N \rightarrow \infty$,

$$\frac{(J_S + J_T - 2)\sinh(v)}{4} = \left(\frac{E}{2 + J_S + J_T} - v\right) \left[\frac{v^2}{2} + \frac{1}{2} \left(\frac{P}{2}\right)^2\right].$$
(15)

The terms with v on the rhs. can be neglected in the limit $P \rightarrow 0$ and we obtain the condition $J_S + J_T - 2 > 0$, which was found in Ref. 4 by solving a two-site problem. The above result seems to imply that the combined excitation also sets the lowest-energy scale for the elementary excitations. However, we show below that it actually never is the lowest one and in the thermodynamic limit either the *SS* or the *TT* (or both) bound states have a lower dispersion in the whole Brillouin zone. The energies of the latter are $E_{SS} = (J_S + 1)\sin^2(P/2)$ and $E_{TT} = (J_T + 1)\sin^2(P/2)$, respectively. The long-wavelength solution for the *ST* excitation follows from Eq. (15):

$$E_{ST} = 2(2+J_S+J_T)\sin^2\left(\frac{P}{4}\right) - \frac{1}{2}\frac{2+J_S+J_T}{(J_S+J_T-2)^2}\left(\frac{P}{2}\right)^8 + \cdots$$

Therefore at small momenta at least one of the splittings of the respective dispersions is always positive:



FIG. 5. Long-wavelength behaviour of the relative amplitude of the symmetric state, $P \ll 1$, for $|J_S - J_T| \neq 0$.

$$E_{ST} - E_{SS} = \frac{1}{2} \left(\frac{P}{2}\right)^2 (J_T - J_S) + \frac{P^4}{384} (6 + 7J_S - J_T) + \cdots,$$
$$E_{ST} - E_{TT} = \frac{1}{2} \left(\frac{P}{2}\right)^2 (J_S - J_T) + \frac{P^4}{384} (6 + 7J_T - J_S) + \cdots.$$

These splittings become larger towards the edge of the Brillouin zone.

It was pointed out above that for the combined excitations the differences due to symmetry of the excited state are much less pronounced than those for the SS excitations. In onedimensional systems such differences are relatively small and vanish very fast in the limit $N \rightarrow \infty$. For instance, the long-wavelength instability of the antisymmetric twomagnon bound state occurs in the region where the so called string hypothesis breaks down (see, e.g., Refs. 8 and 9). The origin of this instability can be explained as follows. The flipped spins tend to be located nearby with a probability distribution decaying with lattice distance. The quantum nature of the excitation allows a formation of an "antibonding" (antisymmetric) state. The nodal point of this state corresponds to large separation of flipped spins. Reaching such a separation becomes possible for a long-wavelength excitation and therefore leads to the dissociation into scattered states.¹⁰ Thus, the critical region is in fact determined by the vanishing of the dynamic interaction, v. However, beyond the critical point these states remain special in the sense that they still conserve some solitonic features even within the band of scattered states. For instance, they have the lowest energy and the most flat dispersion or a "heavier mass," which leads to a sharp density of states. In higher dimensions one expects that such excitations would become resonance states in the limit $N \rightarrow \infty$.^{11,12} The different nature of magnons and orbitons leads to an oscillatory character of the wave function at all momenta. This causes the dynamic interaction to vanish not only at long but also at short wavelengths irrespective of the symmetry. Also for higherdimensional systems only small differences due to symmetry should be expected for an ST excitation. This is in contrast with purely spin excitations, where bound states of different symmetry are well separated in energy.^{11,7} Instead, several closely lying resonances should be observed inside the continuum of scattering states.

IV. DISCUSSION

The exact solution for a finite chain presented above has allowed revelation of several distinctive properties of the combined spin-orbiton excitations that are important for the understanding of their nature. It suggests that in a realistic situation these excitations are more likely to be found in a resonant state within the continuum of scattering states than as true bound states. Despite setting stronger restrictions on the stability of the ordered phase, the combined spin-orbiton excitations have a higher energy and are less stable than excitations of the spin or orbital subsystems. This, however, opens a possibility to probe the orbiton dynamics via excitations of the spin subsystem, e.g., by neutron scattering. Coupling to the orbital degrees of freedom would produce then resonances in the magnon excitation spectrum when the magnon dispersion crosses with the ST resonance. The overall effect of the band of scattering states on the one-magnon

- *On leave from the Institute of Applied Physics, Chişinău, Moldova.
- ¹D.I. Khomskii, Int. J. Mod. Phys. B **15**, 2665 (2001).
- ²E. Saitoh, S. Okamoto, K. T. Takahashi, K. Tobe, K. Yamomoto, T. Kimura, S. Ishihara, S. Maekawa, and Y. Tokura, Nature (London) **410**, 180 (2001).
- ³K. I. Kugel' and D. I. Khomskii, Zh. Éksp. Teor. Fiz. 64, 1429 (1973) [Sov. Phys. JETP 37, 725 (1973)]; Usp. Fiz. Nauk 136, 621 (1982) [Sov. Phys. Usp. 25, 231 (1982)].
- ⁴J. vandenBrink, W. Stekelenburg, D.I. Khomskii, G.A. Sawatzky,

dispersion is yet to be studied. But the exact solution for a discrete chain reveals a qualitative difference of the energy spectrum in such bands as compared to the magnon bands. Interaction in magnon bands produces a uniform shift of noninteracting magnons without changing their structure. The ST bands, on the contrary, undergo a radical change from smooth magnonlike in the absence of interaction to a layered structure with ridge-shaped individual subbands. Such a structure can have a large effect on renormalizing the magnon spectrum, especially at short wavelengths, where oscillations in the wave function and energy dispersion are the largest. The splitting of orbital energy levels due to anisotropy, crystal field, etc., would shift the spectrum of ST excitations to higher energies without changing the intrinsic structure of the bands.

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- and K.I. Kugel, Phys. Rev. B 58, 10 276 (1998).
- ⁵M. Wortis, Phys. Rev. **132**, 85 (1963).
- ⁶M. Karbach and G. Müller, Comput. Phys. **11**, 36 (1997).
- ⁷S. Cojocaru and A. Ceulemans, Phys. Rev. B 66, 224416 (2002).
- ⁸F. Woynarovich, J. Phys. A **15**, 2985 (1982).
- ⁹A.A. Vladimirov, Phys. Lett. A **105**, 418 (1984).
- ¹⁰A. Ceulemans, S. Cojocaru, and L.F. Chibotaru, Eur. Phys. J. B 21, 511 (2001).
- ¹¹R.G. Boyd and J. Callaway, Phys. Rev. **138**, A1621 (1965).
- ¹²M. Hood and P.D. Loly, J. Phys. C **19**, 4729 (1986).