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Crossover from an incommensurate singlet spiral state with a vanishingly small spin gap to a valence-bond solid state in dimerized frustrated ferromagnetic spin chains

Cliò Efthimia Agrapidis,[1] Stefan-Ludwig Drechsler,[1] Jeroen van den Brink,[1,2] and Satoshi Nishimoto[1,2]
[1]*Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany*
[2]*Department of Physics, Technical University Dresden, 01069 Dresden, Germany*

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Motivated by the magnetic properties of the spin-chain compounds $LiCuSbO_4 \equiv LiSbCuO_4$ and $Rb_2Cu_2Mo_3O_{12}$, we study the ground state of the Heisenberg chain with dimerized nearest-neighbor ferromagnetic (FM) ($J_1, J_1' < 0$) and next-nearest-neighbor antiferromagnetic ($J_2 > 0$) couplings. Using the density-matrix renormalization group technique and spin-wave theory, we find a first-order transition between a fully polarized FM and an incommensurate spiral state at $2\alpha = \beta/(1+\beta)$, where α is the frustration ratio $J_2/|J_1|$ and β the degree of dimerization J_1'/J_1. In the singlet spiral state the spin-gap is vanishingly small in the vicinity of the FM transition, corresponding to a situation of $LiCuSbO_4$. For larger α, corresponding to $Rb_2Cu_2Mo_3O_{12}$, and smaller β there is a crossover from this frustration induced incommensurate state to an Affleck-Lieb-Kennedy-Tasaki-type valence-bond solid state with substantial spin gaps.

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Introduction. The exotic phenomena emerged by magnetic frustration have long been fascinating subjects of research in condensed matter physics [1]. Nowadays, quasi-one-dimensional (1D) frustrated systems, despite their simple structure, are at the center of attention as a playground for novel ground states that can emerge from frustration and strong quantum fluctuations due to low dimensionality. So far, various unconventional magnetic states such as quantum spin liquids [2,3], spin-Peierls states [4], and Tomonaga-Luttinger (TL) liquid phases [5] have been investigated. Currently, among the hottest topics are magnetic multipolar and in particular spin-nematic states [6–11] in which magnon bound states are formed from a subtle competition between geometrical balance of ferromagnetic (FM) and antiferromagnetic (AFM) correlations among spins.

Very recently, a magnetic field-induced "hidden" spin-nematic state was reported in the anisotropic frustrated spin-chain cuprate $LiCuSbO_4$ [12]. By the nuclear magnetic resonance technique, a field-induced spin gap was observed above a field ~13 T in the measurements of the ^{7}Li spin relaxation rate T_1^{-1}, supported by static magnetization and electron spin resonance data. This material has a unique crystal structure. In the CuO_2 chain, four nonequivalent O^{2-} ions within a CuO_4 plaquette give rise to two kinds of nonequivalent left and right Cu-Cu bonds along the chain direction. This gives rise to alternating nearest-neighbor transfer integrals ($t_1 \neq t_1'$). As a result, a sizable splitting of the two nearest-neighbor FM exchange integrals was estimated: $J_1 \approx -160$ K and $J_1' \approx -90$ K, whereas the next-nearest-neighbor AFM coupling is $J_2 \approx 37.6$ K [see Fig. 1(a)]. Another example of a FM dimerized chain compound is $Rb_2Cu_2Mo_3O_{12}$, which has CuO_2 ribbon chains. Here, its ribbon chains are twisted, so that the Cu-Cu distances and the Cu-O-Cu angles are slightly alternating. Accordingly, a small dimerization of the nearest-neighbor exchange integrals is expected. Assuming no dimerization, the values of the FM nearest- and AFM next-nearest-neighbor exchanges have been estimated as -138 and 51 K, respectively, by the fitting of susceptibility and magnetization [13]. Besides, a nonmagnetic ground state with energy gap $E_g \sim 1.6$ K has been experimentally detected [14]. So far, the 1D dimerized AFM Heisenberg has been extensively studied in connection to the celebrated spin-Peierls compound $CuGeO_3$ [15]. In contrast, the dimerized FM case has been hardly ever discussed. Recently, only the weakly dimerized case has been investigated [16], and theoretical studies are definitely required.

Motivated by the above observations, we study a dimerized FM Heisenberg chain with next-nearest-neighbor AFM couplings by using the spin-wave theory (SWT) and the density-matrix renormalization group (DMRG) method. The ground-state phase diagram is obtained as a function of dimerization and frustration strengths, based on the numerical results of total spin, spin gap, spin-spin correlation function, and Tomonaga-Luttinger (TL) liquid exponent. We establish the presence of a frustration induced incommensurate singlet state with a spin gap that is vanishingly small close to the vicinity to a first-order FM transition, corresponding to the situation of $LiCuSbO_4$. Despite the vanishingly small gap, correlation lengths are comparable to those in the large-gap region in the phase diagram. For larger α and smaller β, there is a crossover from this frustration induced incommensurate state to an Affleck-Lieb-Kennedy-Tasaki (AKLT)-type valence-bond solid (realized at $\beta = 0$) with substantial spin gaps. We also confirm the presence of a finite spin gap in the uniform J_1-J_2 limit.

Model and method. Our spin Hamiltonian is given by

$$H = J_1 \sum_{i=\text{even}} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_1' \sum_{i=\text{odd}} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}, \tag{1}$$

where $\mathbf{S}_i$ is a spin-1/2 operator at site i. The nearest-neighbor ($J_1, J_1' < 0$) and next-nearest-neighbor ($J_2 > 0$) interactions are FM and AFM, respectively [see Fig. 1(a)], and we use the notations of next-nearest-neighbor coupling ratio $\alpha = J_2/|J_1|$ and nearest-neighbor coupling ratio $\beta = J_1'/J_1$ hereafter.

When the system is undimerized ($\beta = 1$), we are dealing with the so-called J_1-J_2 model. Increasing α, a phase with incommensurate spin-spin correlations follows a FM phase. The transition occurs at $\alpha = 1/4$, both in the quantum as

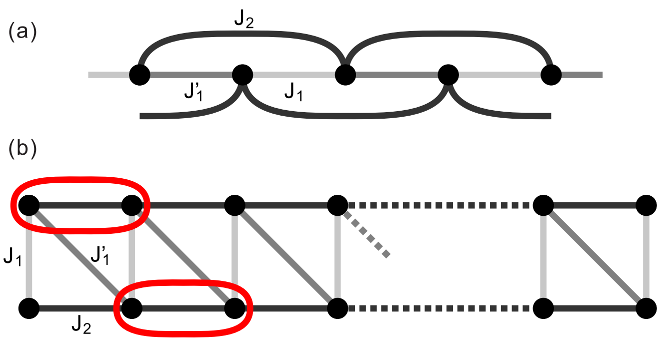

FIG. 1. (a) Lattice structure of the J_1- J_1'-J_2 model. (b) Topologically equivalent situation which allows for a schematic picture of the valence-bond-solid gapped state. Red ellipses indicate spin-singlet pairs that form in the AKLT (Haldane) state.

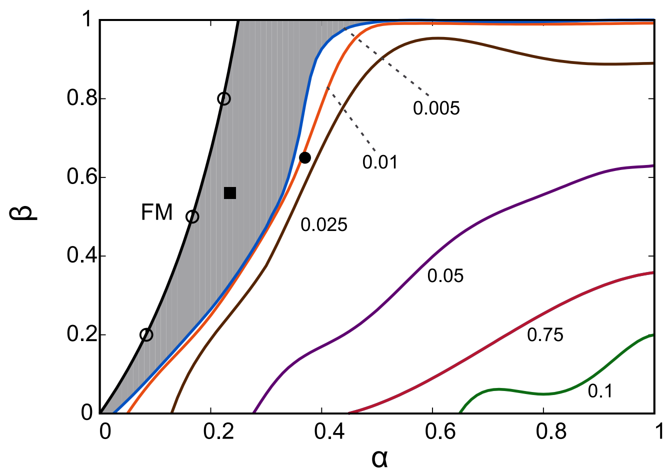

FIG. 2. Phase diagram of the J_1-J_1'-J_2 model in the α-β plane. Contour map for the spin gap $\Delta/|J_1|$ is shown. The black line represents the boundary of the fully polarized ferromagnetic and gapped incommensurate spiral states, obtained by spin-wave theory. The open circles mark the results from DMRG. The shaded area indicates the region with a vanishingly small gap ($\Delta|J_1| < 10^{-3}$). Filled circle and square indicate the locations of $Rb_2Cu_2Mo_3O_{12}$ and $LiCuSbO_4$, respectively.

well as in the classical model [17,18]. The incommensurate ("spiral") correlations are short ranged in the quantum model [19,20]. A vanishingly small gap was predicted by the field-theory analysis [21] but no numerical evidence exists so far. In the limit of $\beta = 0$, the system (1) is equivalent to spin ladder with AFM legs and FM rung couplings. Since this system can be effectively reduced to an $S = 1$ AFM Heisenberg chain with regarding two $S = 1/2$ spins on each rung as a $S = 1$ spin [23,24], the ground state is gapped as predicted by the Haldane conjecture [22]. Therefore the ground state can be well described by a valence-bond-solid (VBS) picture, proposed in the AKLT model [25]. The schematic picture is shown in Fig. 1(b).

The DMRG method [26] is employed to investigate the ground-state properties of the system (1). We calculate the total spin with periodic boundary conditions, and spin gap, spin-spin correlation functions, and the Tomonaga-Luttinger (TL) spin exponent with open boundary conditions. We keep up to $m = 6000$ density-matrix eigenstates in the renormalization procedure and extrapolate the calculated quantities to the limit $m \to \infty$ if necessary. Furthermore, several chains with lengths up to $L = 800$ are studied to handle the finite-size effects. In this way, we can obtain quite accurate ground states within the error of $\Delta E/L = 10^{-9} - 10^{-10}|J_1|$.

Ferromagnetic critical point. In the limit of $\beta = 0$ and $\alpha = 0$, the FM critical point no longer exists because the system is solely composed of isolated spin-triplet dimers. However, if β is finite, the FM order is expected for small α. Let us then consider the β dependence of the critical point. Since the quantum fluctuations vanish at the FM critical point, the classical SWT may work perfectly for estimating the FM critical point. According to SWT, the excitation energy for a FM ground state is given as $2\omega_q = -\sqrt{1+\beta^2+2\beta\cos(2q)} + 2\alpha\cos(2q)$. The system is in the FM ground state if $\omega_q > 0$ for all q; otherwise, it is in the spiral singlet state. Thus the FM critical point is derived as

$$\alpha_{c,1} = \frac{\beta}{2(1+\beta)}. \tag{2}$$

As shown in Fig. 2, the FM region is simply shrunk with decreasing β, and disappears in the limit of $\beta = 0$ as a consequence of isolated FM dimers. It can be numerically confirmed by calculating the ground-state expectation value of the total-spin quantum number S of the whole system, $\boldsymbol{S}^2$ (see Ref. [27]).

Haldane gapped state. So far, the spin gapped state has been verified in the limit of $\beta = 0$ [23,24]. This can be interpreted as a realization of the AKLT VBS state. However, it is a nontrivial question what happens to the spin gap for finite β. In our DMRG calculations, the spin gap Δ is evaluated as the energy difference between the lowest triplet state and the singlet ground state,

$$\Delta(L) = E_0(L,S^z=1) - E_0(L,S^z=0),\ \Delta = \lim_{L\to\infty}\Delta(L), \tag{3}$$

where $E_0(L)$ is the ground-state energy for a given number of system length L and z component of total spin S^z.

First, we focus on the case of $\beta = 0$, namely, a ladder consisting of two AFM leg chains and FM rungs. In Fig. 3(a), the extrapolated values of $\Delta/|J_1|$ are plotted as a function of α. The gap opens at $\alpha = 0$ and increases monotonously with increasing α, and saturates at a certain value scaled by $|J_1|$. This means that Δ is finite for all α at $\beta = 0$, which is consistent with the prediction by the bozonization method [24] and the conformal field theory [28]. In the limit of $\alpha = 0$ the system is exactly reduced to a $S = 1$ AFM Heisenberg chain:

$$H_{\rm eff} = J_{\rm eff}\sum_i \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1} - J_1 L/4, \tag{4}$$

where $\tilde{\mathbf{S}}_i$ is a spin-1 operator as a resultant spin $\tilde{\mathbf{S}}_i = \mathbf{S}_{2i} + \mathbf{S}_{2i+1}$ and $J_{\rm eff} = J_2/2$. In the inset of Fig. 3(a), Δ is replotted in units of α. We obtain $\Delta/J_2 = 0.2045$ in the limit $\alpha = 0$. The Haldane gap of the system (4) has been calculated as $\Delta/J_{\rm eff} = 0.410479$ [29]. Thus we can confirm $J_{\rm eff} = J_2/2$ numerically for the mapping from Eq. (1) to Eq. (4) at the limit $|J_1|/J_2 (= 1/\alpha) \to 0$ and $\beta = 0$.

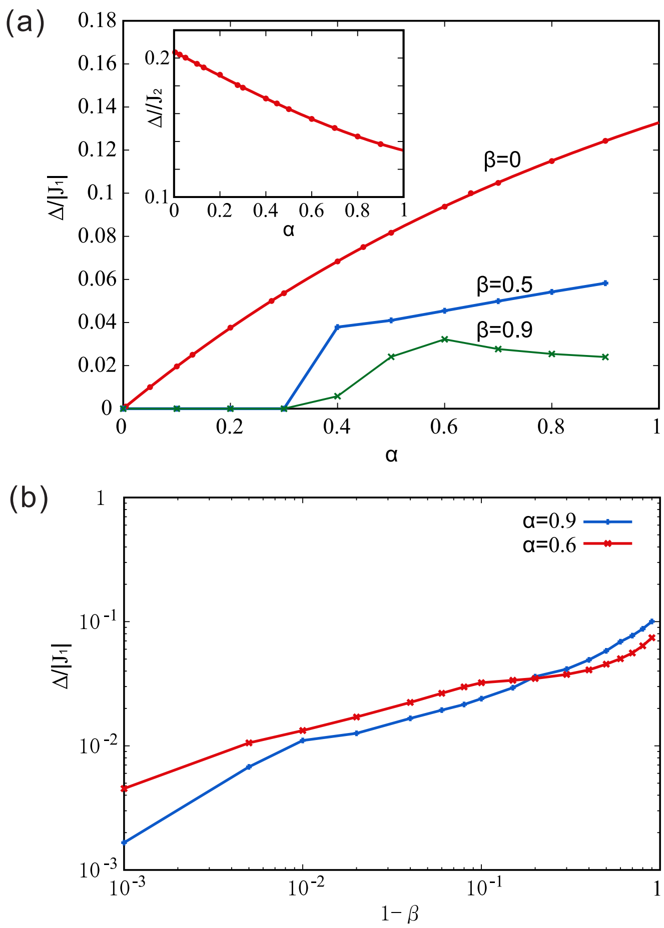

FIG. 3. (a) Extrapolated spin gap $\Delta/|J_1|$ as a function of α for $\beta = 0, 0.5$, and 0.9. Inset: similar plot of Δ/J_2 at $\beta = 0$. (b) Log-log plot of $\Delta/|J_1|$ as a function of $1-\beta$ for $\alpha = 0.6$ and 0.9.

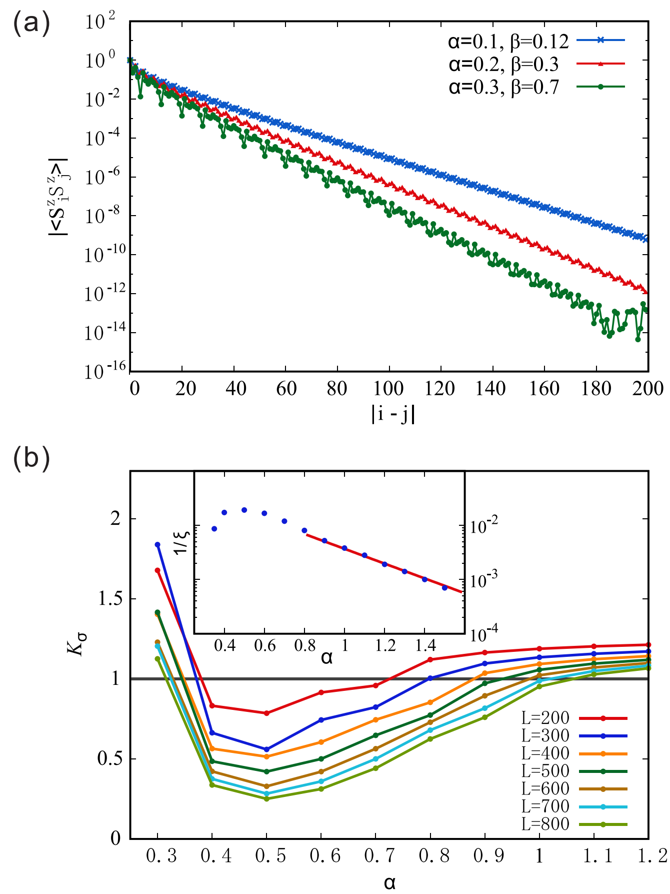

FIG. 4. (a) Equal-time spin-spin correlation function $|\langle S_i^z S_j^z\rangle|$ as a function of distance $|i-j|$ at $\alpha = 0.1, \beta = 0.12$, $\alpha = 0.2, \beta = 0.3$, and $\alpha = 0.3, \beta = 0.7$ for the $L = 400$ cluster. (b) Tomonaga-Luttinger liquid spin exponent as a function of α for systems with several lengths $L = 200$–800. Inset: inverse correlation length $1/\xi$ as a function of α. The solid line shows a fitting by by $1/\xi = 0.085\exp(-\pi\alpha)$.

Next, we look at the effect of β on the spin gap. Figure 3(b) shows a log-log plot of $\Delta/|J_1|$ as a function of $1-\beta$ for $\alpha = 0.6$ and 0.9. The behaviors are nontrivial but Δ decays roughly as a power law with decreasing $1-\beta$. As a result, the gap is vanishingly small near the uniform $J_1 - J_2$ limit ($\beta \sim 1$). Besides, it is interesting that Δ for $\alpha = 0.6$ is larger than that for $\alpha = 0.9$ at larger β and opposite at smaller β, which may suggest that the gapped state near $\beta = 1$ is no longer the AKLT-type VBS state but the frustration induced one (see below). This is consistent with a maximun gap around $\alpha = 0.6$ at weak dimerization ($\beta = 0.9$). On the other hand, an adiabatic connection of the AKLT-type VBS state from $\beta = 0$ to 1 was predicted by the field-theoretical analysis for $|J_1| \ll J_2$ [30]. A contour plot of the magnitude of Δ is given in Fig. 2. We can see a rapid decay of Δ with approaching the FM phase. However, Δ is too small to figure out whether it remains finite, e.g., $\Delta \lesssim 10^{-3}$, in the vicinity of the FM critical boundary. Therefore, to verify the presence or absence of the gap, we checked the asymptotic behavior of spin-spin correlation function $|\langle S_i^z S_j^z\rangle|$. In Fig. 4(a), the semilogarithmic plot of $|\langle S_i^z S_j^z\rangle|$ as a function of distance $|i-j|$ is shown for some parameters near the FM critical boundary. The distances $|i-j|$ are taken about the midpoint of the systems to exclude the Friedel oscillations from the system edges, i.e., $(i+j)/2$ locates around the midpoint of the systems. All of them exhibit exponential decay of $|\langle S_i^z S_j^z\rangle|$ with distance, which clearly indicates the presence of a finite spin gap. The curves are well-fitted with the expression $|\langle S_i^z S_j^z\rangle| \propto \cos[Q(i-j)]|i-j|^{-\frac{1}{2}}e^{-\frac{|i-j|}{\xi}}$ for long distances [31,32]; the correlation lengths ξ are estimated as $\xi = 11.6$ ($\alpha = 0.1, \beta = 0.12$), $\xi = 8.6$ ($\alpha = 0.2, \beta = 0.3$), and $\xi = 7.3$ ($\alpha = 0.3, \beta = 0.7$). In the AFM $J_1 - J_2$ model [31], a region with $\xi \approx 10$ still has a spin gap of order of $10^{-1}J_1$. This may imply the spin velocity of our system is more than two digits smaller than that of the AFM J_1-J_2 model since $\Delta = v_s/\xi$, where v_s is the spin velocity.

Uniform J_1-J_2 model. In the uniform case ($\beta = 1$) the existence of a tiny gap for $\alpha \gtrsim 3.3$ was predicted by the field-theory analysis [21]. However, the investigation for smaller α is lacking. Therefore, to verify the presence or absence of a gap at smaller α, we investigated the TL liquid spin exponent K_σ. For our system having four Fermi points $(\pm k_{F1}, \pm k_{F2})$, we here assume the asymptotic behavior of the spin-spin correlation function to be a power-law decay, like

$$\langle S_0^z S_r^z\rangle \sim -\frac{K_\sigma}{2\pi^2 r^2} + \frac{A\cos[2(k_{F1}-k_{F2})r]}{r^{2K_\sigma}} + \cdots, \quad (5)$$

in analogy with the case of two coupled chains [33], because the low-energy excitation spectra are similar to those of our model [34]. By summing up (5) over the distance, we obtain

$$K_\sigma = \lim_{L\to\infty} \frac{L}{2} \sum_{kl} e^{i\frac{2\pi}{L}(k-l)} \langle S_k^z S_l^z \rangle. \tag{6}$$

The value of $K_\sigma = 0$ indicates a spin-gapped state with an exponential decay of the spin-spin correlation in real space, whereas the convergence to a finite value of K_σ in the thermodynamic limit suggests a spin-gapless state with the power-law decay ($K_\sigma = 1$ within the TL liquid theory) [35]. In Fig. 4(b), K_σ is plotted as a function of α for several chain lengths. We clearly find a region where K_σ approaches 0 with increasing system size. This clearly indicates the existence of a gapped state [36,37]. The fastest convergence to $K_\sigma \to 0$ around $\alpha = 0.5$–0.6 may imply the maximum gap there, similarly to the case of AFM J_1-J_2 chain. For $\alpha > 1$, K_σ may seem to converge to $K_\sigma = 1$. Nevertheless, the validity of the TL liquid theory is not straightforward around $J_2/|J_1| \sim 1$, and it is also difficult to exclude the logarithmic corrections for the small-gap region. Therefore, to consider the connection to the gapped state with tiny gap $\Delta \lesssim 10^{-40} J_2$ at $\alpha > 3.3$ predicted by the field theory [21], we estimated the correlation length from the fitting of spin-spin correlation by a fitting function $\langle S_0^z S_r^z \rangle = A \exp(-r/\xi)$, where ξ is the correlation length (see Supplemental material). In the inset of Fig. 4(b), the inverse correlation length is plotted as a function of α. We found that the inverse correlation length is well fitted by $1/\xi = 0.085 \exp(-\pi\alpha)$ for large α. Since $\Delta = v_s/\xi$, it may be feasible to speculate that the gap has a maximum around $\alpha = 0.5 - 0.6$, decreases with increasing α, and smoothly connects to the tiny gap region.

Finally, let us explicitly address the relevance of the calculations above for the two spin-chain materials mentioned in Introduction. For $LiCuSbO_4$, $\alpha = 0.235$ and $\beta = 0.56$ are estimated from the density-functional calculations: $J_1 \approx -160$ K, $J_1' \approx -90$ K, and $J_2 \approx 37.6$ K [12,38]. The system is in the gapped spiral state, but very close to the FM phase where the spin-gap is vanishingly small. Thus the spin gap may be too small to be detected experimentally. The second compound is $Rb_2Cu_2Mo_3O_{12}$. If we use the previously estimated parameters $J_1 = -138$ K and $J_2 = 51$ K ($\alpha = 0.37$), a substantial dimerization ($\beta = 0.65$) of J_1 and J_1' is necessary to reproduce the experimentally observed gap $E_g \sim 1.6$ K, namely, $J_1 = -138$ K and $J_1' = -90$ K. Furthermore, if it is more appropriate to consider the value -138 K as an averaged FM coupling $(J_1 + J_1')/2$, then an even larger dimerization would be needed. In practice, the actual J_1 should be somewhat smaller or J_2 should be larger. A detailed analysis of the experimental data that explicitly takes into account the dimerization can clarify this point. In the context of these two compounds and also in general, the influence of an external magnetic field is of considerable interest and will be addressed elsewhere.

Conclusion. We considered a frustrated J_1-J_2 spin chain with/without dimerization of nearest-neighbor FM coupling and determined its phase diagram. The FM critical point was analytically determined to be $\alpha_c = (\beta/2)/(1+\beta)$ by applying the linear spin-wave theory, which was confirmed by the numerical calculation of the total spin. The transition between the fully polarized FM and the singlet spiral states is of the first order and no partially polarized FM state exists. The spin-gap in the vicinity of the FM boundary was confirmed to be finite by the exponential decay of the spin-spin correlation functions but it is vanishingly small. In the uniform J_1-J_2 chain, the gapped state appears at least around $\alpha \sim 0.5$–0.6 where the TL liquid exponent K_σ goes to 0 in the thermodynamic limit. Near $\beta = 0$, the spin-gap increases with increasing α; whereas, near $\beta = 1$, it has a maximum value around the strongest frustration region $\alpha = 0.5$–0.6. Therefore the gap opening in the entire incommensurate singlet phase may be interpreted as a crossover from the AKLT-type valence-bond solid state near $\beta = 0$ to the frustration-induced dimerized state near $\beta = 1$.

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[38] Thereby fixed FM contributions to the total J_1 and J_1' values have been assumed, i.e., taking into account the modification of the AFM superexchange contributions to the former, only. An LDA+U analysis available in future might provide somewhat refined numbers. Within a pd-multiband Hubbard model this corresponds to fixed direct ferromagnetic exchange interactions K_{pd} and ferromagntic Goodenough-Kanamori exchange interactions involving the Hund's rule coupling involving the intermediate oxygen sites generic for edge-shared CuO_2 chain compounds. The latter might be checked by advanced quantum chemistry calculations for small chain clusters. In the absence of results of such calculations at present, the model considered here provides a convenient tool to investigate phenomenologically $LiSbCuO_4$ and other related compounds.