Spin Gap and String Order Parameter in the Ferromagnetic Spiral Staircase Heisenberg Ladder: A Quantum Monte Carlo Study

C. Brünger,[1] F. F. Assaad,[1] S. Capponi,[2] F. Alet,[2] D. N. Aristov,[3,4,*] and M. N. Kiselev[5]

[1]Institut für Theoretische Physik, Universität Würzburg, D-97074 Würzburg, Germany
[2]Laboratoire de Physique Théorique, IRSAMC, Université Paul Sabatier, CNRS, 31062 Toulouse, France
[3]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Germany
[4]Center for Functional Nanostructures, Universität Karlsruhe, 76128 Karlsruhe, Germany
[5]The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, Trieste, Italy

(Received 20 June 2007; published 7 January 2008)

We consider a spin-$1/2$ ladder with a ferromagnetic rung coupling $J_\perp$ and inequivalent chains. This model is obtained by a twist (θ) deformation of the ladder and interpolates between the isotropic ladder ($\theta = 0$) and the $SU(2)$ ferromagnetic Kondo necklace model ($\theta = \pi$). We show that the ground state in the (θ, $J_\perp$) plane has a finite string order parameter characterizing the Haldane phase. Twisting the chain introduces a new energy scale, which we interpret in terms of a Suhl-Nakamura interaction. As a consequence we observe a crossover in the scaling of the spin gap at weak coupling from $\Delta/J_\parallel \propto J_\perp/J_\parallel$ for $\theta < \theta_c \simeq 8\pi/9$ to $\Delta/J_\parallel \propto (J_\perp/J_\parallel)^2$ for $\theta > \theta_c$. Those results are obtained on the basis of large scale quantum Monte Carlo calculations.

DOI: 10.1103/PhysRevLett.100.017202 PACS numbers: 75.10.Pq, 71.10.Fd, 73.22.Gk

Low-dimensional quantum magnets are fascinating objects from both experimental and theoretical points of view. Spin-$1/2$ ladders have been widely studied and interpolate between the physics of one-dimensional antiferromagnetic (AF) spin chains and two-dimensional systems [1]. In the one-dimensional (1D) case, there is an important mapping between spin-$1/2$ Heisenberg AF chains and Luttinger liquids [2] which allows to treat such chains by means of exact fermionization and bosonization methods, resulting in a well-understood gapless phase [3]. Coupling identical chains to form a spin ladder is, however, not a trivial task from a theoretical point of view [4,5]. Indeed, the coupling is a relevant perturbation and, up to logarithmic corrections, opens a gap proportional to the interchain coupling $J_\perp$ [6,7]. In this Letter, we consider the case of two *inequivalent* chains coupled with a ferromagnetic rung coupling $J_\perp < 0$. By using quantum Monte Carlo (QMC) techniques we (i) demonstrate the existence of a finite spin gap, characteristic of a Haldane phase, and (ii) observe the emergence of a new energy scale at weak coupling. This latter energy scale, which we interpret as a Suhl-Nakamura interaction [8], appears only when the exchange energies of each chain strongly differ. When the spin velocity on one of the legs vanishes, the bosonization fails since a simple formulation of the continuum limit on which this approach relies [6] is inhibited. This regime requires high-precision unbiased numerical simulations.

The model that we consider is dubbed the Spiral Staircase Heisenberg Ladder:

$$\hat{H} = J_\parallel \sum_i [\hat{\mathbf{S}}_{1,i} \cdot \hat{\mathbf{S}}_{1,i+1} + \cos^2(\theta/2)\hat{\mathbf{S}}_{2,i} \cdot \hat{\mathbf{S}}_{2,i+1}] + J_\perp \sum_i \hat{\mathbf{S}}_{1,i} \cdot \hat{\mathbf{S}}_{2,i}. \quad (1)$$

Here $\hat{\mathbf{S}}_{\alpha,i}$ is a spin-$1/2$ operator on leg α and lattice site i. $J_\parallel > 0$ sets the energy scale and the interchain coupling is taken to be ferromagnetic $J_\perp < 0$. Geometrically, this model may be interpreted as a result of twist deformation of a 2-leg ladder [Fig. 1(a)] with twist performed along one of the legs. Such a spiral structure is characterized by the angle θ [see Fig. 1(b)] and interpolates between the isotropic ladder ($\theta = 0$) and a ferromagnetic $SU(2)$ Kondo Necklace [9] model ($\theta = \pi$) [10–13]. A motivation to study this specific geometry comes from the fact that a realization of the model schematically presented in Fig. 1(c) was synthesized as a stable organic biradical crystal PNNNO [14]. Possible candidates for realizations with twist angle $0 < \theta < \pi$ might be found in the families of molecular chains decorated by magnetic radicals.

In the strong coupling limit, $|J_\perp/J_\parallel| \gg 1$, the model maps onto the spin-1 Heisenberg chain with effective

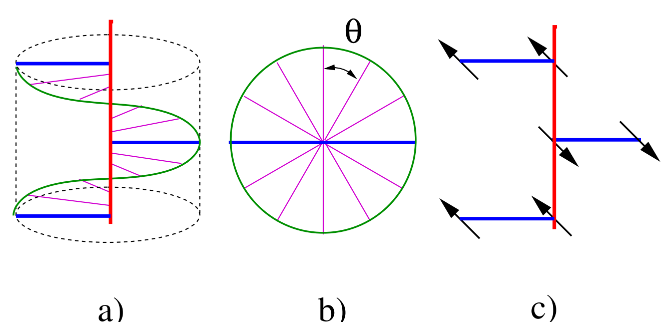

FIG. 1 (color online). (a) Sketch of Spiral Staircase Heisenberg Ladder. (b) View of the model from the top. (c) For $\theta = \pi$, the model maps to the 1D $SU(2)$ ferromagnetic Kondo necklace model [9].

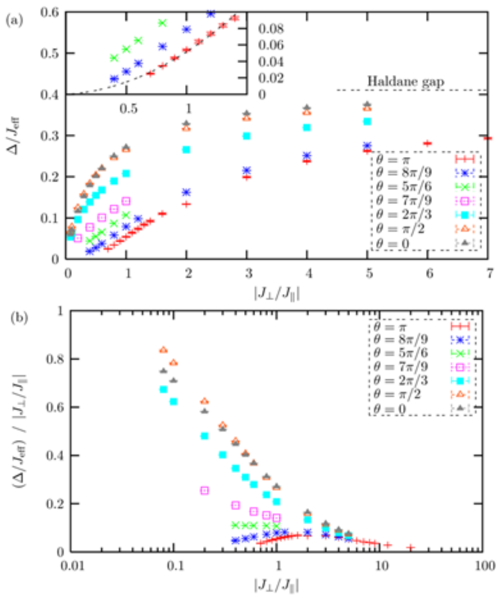

FIG. 2 (color online). (a) Spin gap $\Delta(J_\perp)$ as a function of $|J_\perp/J_\parallel|$ for different twist angles θ. The gap is rescaled by $J_{\rm eff} = \frac{J_\parallel}{4}[1 + \cos^2(\theta/2)]$ such that in the large-$|J_\perp|$ limit, it converges asymptotically toward the Haldane gap of a spin-1 chain. At weak couplings, we have carried out QMC simulations up to $\beta J_\parallel = 2500$ and 2×512 spins to ensure size and temperature convergence. Inset: zoom on the weak-coupling region. (b) Results for spin gap on a semilogarithmic scale.

exchange interaction $J_{\rm eff} = \frac{J_\parallel}{4}[1 + \cos^2(\theta/2)]$. This phase has a spin gap [15] given by $\Delta_H/J_{\rm eff} = 0.41048(6)$ [16] and is qualitatively grasped by the valence bond solid (VBS) wave function of Affleck *et al.* [17]. This VBS state has a hidden antiferromagnetic order [18] which is picked up by the nonlocal string order parameter [19] (see a recent discussion in [20]):

$$\langle \hat{\mathcal{O}}_s(n)\rangle = \left\langle \hat{S}^z_{n_0} \exp\left[i\pi \sum_{j=n_0}^{n_0+n} \hat{S}^z_j \right] \hat{S}^z_{n_0+n} \right\rangle \qquad (2)$$

with $\hat{S}^z_j = \hat{S}^z_{1,j} + \hat{S}^z_{2,j}$. At weak couplings, the analysis depends on the twist angle θ. For small twist angles (i.e., close to the isotropic case), one can rely on the bosonization and numerical results of Refs. [6,7] which yield a spin gap proportional to $|J_\perp|$ up to logarithmic corrections. On the other hand, at $\theta = \pi$ the spin velocity on the second leg vanishes thus inhibiting the very starting point of Ref. [6]. Alternative approaches such as a mean-field theory based on a Jordan-Wigner transformation, which yields the correct result for the isotropic ladder, predicts a spin gap $\Delta \propto J_\perp^2/J_\parallel$ at $\theta = \pi$ [21]. A flow equation calculation has recently been carried out for the $SU(2)$ Kondo necklace model [22] [i.e., $\theta = \pi$ in Eq. (1)] and is interpreted in terms of the onset of a spin gap irrespective of the value of $J_\perp/J_\parallel$. Note that in this analytical approach, the conclusion about the existence of the spin gap at small $J_\perp/J_\parallel$ subtly depends on the treatment of the energy cutoff. Moreover, this method cannot predict the scaling of the spin gap in this weak-coupling regime.

To disentangle this situation, we have performed large scale QMC simulations of the ferromagnetic spiral staircase model. Two variants of the loop algorithm [23] were applied. For the string order parameter and the spin-spin correlation functions, we used a discrete time algorithm and extract the spectral functions via stochastic analytical continuation schemes [24,25]. For the spin gap calculation, a continuous time loop algorithm was used, where the gap is calculated by a second moment estimator of the correlation length [16].

Our results for the spin gap in units of $J_{\rm eff}$ in the $(\theta, J_\perp)$ plane are plotted in Fig. 2. Enhancing the twist angle from $\theta = 0$ to $\theta = \pi/2$ leaves the spin gap, measured in units of $J_{\rm eff}$, next to invariant thereby showing that a *small* twist is an irrelevant perturbation [26]. For larger values of θ, Δ is suppressed, and in the limit $\theta = \pi$ the approach to the Haldane value in the limit $J_\perp \to -\infty$ is surprisingly slow. At small values of $|J_\perp/J_\parallel|$, and $\theta = 0$ we reproduce the results of Ref. [7], namely, $\Delta \propto J_\perp$ [see Fig. 2(b)]. Here and in what follows, we neglect logarithmic corrections in our discussion. Figure 2(b) shows that this weak-coupling behavior of the spin gap is sustained up to $\theta < \theta_c \simeq 8\pi/9$. Beyond this critical angle [27], the data allow for different interpretations. Let us concentrate on the twist angles $\theta = 8\pi/9$ and $\theta = \pi$. A linear extrapolation of the data would lead to the vanishing of the spin gap at a finite critical value of $J_\perp$. However, in this parameter range, we find a finite string order parameter (see below), incompatible with a gapless phase. As suggested by a Jordan-Wigner mean-field analysis [21], we instead assume the existence of an inflection point and fit the data to a quadratic form in the limit $J_\perp \to 0$ [see inset of Fig. 2(a)]. Let us note, however, that we cannot exclude the possibility of an exponential scaling.

The scaling of the spin gap at $\theta > \theta_c$ implies a rapid increase of the spin correlation length $\xi \propto J_\parallel/\Delta$. For $\theta = \pi$ and $J_\perp/J_\parallel = -0.5$, spin correlations decay exponentially with characteristic length scale $\xi \simeq 115$ (see Fig. 3). At $J_\perp/J_\parallel = -0.3$ no sign of exponential decrease is apparent on the considered 2×800 lattice. This is consistent with a spin gap decreasing as $J_\perp^2/J_\parallel$ (or faster). Indeed, such a scaling leads to $\xi \geq 300$ which is comparable to the largest distance $L/2 = 400$ accessible in our simulation of a 2×800 lattice.

On length scales $|i - j| < \xi$ the spin-spin correlation functions follow a slow power law. In particular, the data of Fig. 3 at $J_\perp/J_\parallel = -0.3$ are consistent with $S(|i - j|) \propto (-1)^{|i-j|}|i - j|^{-1/3}$. At $\theta = \pi$, the effective interaction on the second leg is set by the Suhl-Nakamura (SN) [28] interaction [8]. In second order perturbation theory, without attempting any self-consistent calculation, this interaction takes the form $J_{\rm SN}(q) \propto J_\perp^2 \chi_s(q, \omega = 0)$ in Fourier space. Here, $\chi_s(q, \omega = 0)$ is the spin susceptibility of the spin-1/2 chain. A first step towards a self-consistent treat-

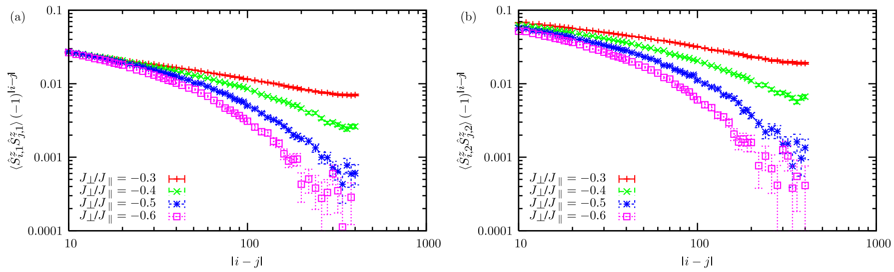

FIG. 3 (color online). Spin-spin correlation function (a) on the first leg and (b) on the second leg for the Kondo necklace model ($\theta = \pi$) at different couplings $J_\perp/J_\parallel$ on a 2×800 lattice. Simulations are carried out at $\beta J_\parallel = 7000$ ($J_\perp/J_\parallel = -0.3, -0.4$), $\beta J_\parallel = 5000$ ($J_\perp/J_\parallel = -0.5$), and $\beta J_\parallel = 2000$ ($J_\perp/J_\parallel = -0.6$).

ment is to allow for a gap, Δ, in $\chi_s(q, \omega = 0)$. Thereby and in real space we expect SN interaction to have a range set by ξ. We interpret the above mentioned very slow decay of the spin-spin correlations on both legs and on a length scale set by ξ as a consequence of the SN interaction. The SN interaction at $\theta = \pi$ sets a new low-energy scale in the problem, corresponding to the slow dynamics of the spin degrees of freedom on the second leg. Because of the ferromagnetic coupling between the chains, this slow dynamics will equally dominate the low-energy physics of the spins on the first chain. This new energy scale is also apparent in the dynamical spin structure factor $S(q, \omega)$ plotted in Fig. 4. As is apparent, a narrow magnon band emerges as the angle θ grows from 0 to π. To lend support to the interpretation in terms of the SN interaction, we have checked with exact diagonalization methods that the width of the magnon band at $\theta = \pi$ indeed scales as $J_\perp^2/J_\parallel$ in the weak interleg coupling limit (data not shown). In the vicinity of $\theta = \pi$, we hence expect that the low-energy effective model is given by a spin-1 Heisenberg chain with exchange coupling set by the SN interaction. Assuming the validity of this low-energy model, we predict a spin gap which scales as $J_{\rm SN} \propto J_\perp^2/J_\parallel$.

The above arguments and data suggest that irrespective of the twist angle and coupling $J_\perp$, the ground state of the model corresponds to the Haldane phase.

We confirm this point of view by computing the string order parameter $\mathcal{O}_s = \langle \hat{\mathcal{O}}_s(n) \rangle|_{n=L/2}$ on a 2×800 lattice [see Fig. 5(a)], which is finite in the Haldane phase [19]. Strictly speaking, this is not a sufficient condition to ascertain the Haldane physics since we also need to show that $\mathcal{O}_H = \langle \exp[i\pi \sum_{j=n_0}^{n_0+n} \hat{S}_j^z] \rangle|_{n=L/2}$ vanishes in the thermodynamic limit (when both $\mathcal{O}_s > 0$ and $\mathcal{O}_H > 0$, an Ising order is present [19]). In the region where the correlation length ξ exceeds the lattice length, finite-size effects are present (see caption of Fig. 5). In particular, when the lattice size is smaller than the correlation length, both $\mathcal{O}_H$ and $\mathcal{O}_s$ take nonzero values, since the very slow decay of the spin correlations mimics Ising-type order. As the system size grows beyond the correlation length, $\mathcal{O}_H$ decreases exponentially whereas $\mathcal{O}_s$ in enhanced. Those size effects are explicitly shown in Fig. 5(b) at $J_\perp/J_\parallel = -0.2$, $\theta = 8\pi/9$ where $L \gg \xi$ and $J_\perp/J_\parallel = -0.3$, $\theta = \pi$ where our maximal system size barely exceeds the estimated correlation length. Taking those size effects into account, we conclude that in the thermodynamic limit, only the string order parameter $\mathcal{O}_s$ is finite in the whole $(\theta, J_\perp)$ plane.

In conclusion, we have established that the ferromagnetic spiral staircase is in a Haldane phase, irrespective on the twist θ and coupling constant $J_\perp$. In the weak-coupling region, twisting the ladder introduces a new low-energy scale which we interpret in terms of a SN interaction. As a consequence and for $\theta > \theta_c \sim 8\pi/9$, we have provided numerical data showing that at weak coupling, the spin gap decreases faster than the linear $J_\perp$ behavior of the 2-leg ladder ($\theta = 0$). Analysis of the data is consistent with the picture that, for $\theta \geq \theta_c$, the spin gap tracks the SN scale and is hence proportional to $J_\perp^2/J_\parallel$.

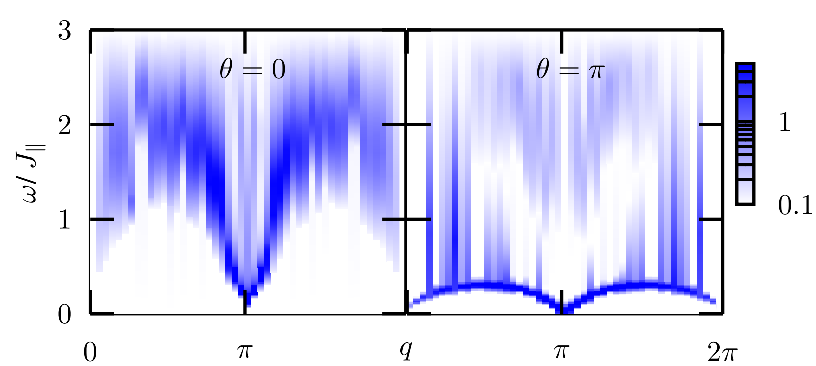

FIG. 4 (color online). Dynamical spin-spin correlations at $J_\perp/J_\parallel = 1$ for the ladder system ($\theta = 0$) and the Kondo necklace model ($\theta = \pi$). Here we consider a bonding combination of the spins across the rungs ($\beta J_\parallel = 200$, $L = 100$).

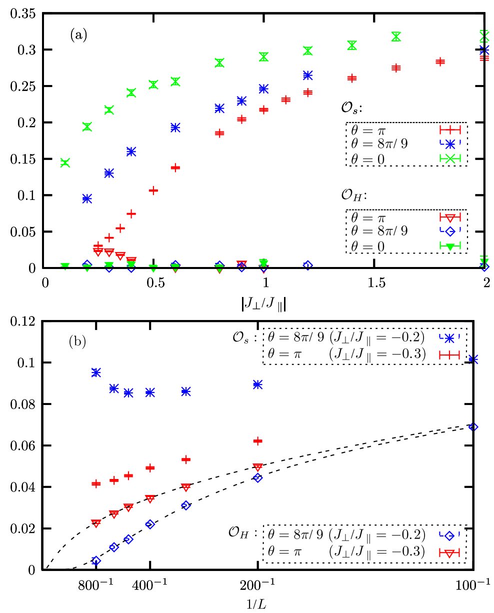

FIG. 5 (color online). (a) String order parameter $\mathcal{O}_s$ and $\mathcal{O}_H$ as a function coupling $J_\perp/J_\parallel$ and several twist angles. For $\theta = 8\pi/9$, π finite-size effects are still present for the considered $L = 800$ lattice in the parameter range $|J_\perp/J_\parallel| < 0.5$. For $|J_\perp/J_\parallel| > 1.0$ the system size $L = 400$ is sufficiently large enough to guarantee convergence. Simulations are carried out up to $\beta J_\parallel = 7000$. (b) Finite-size scaling of the order parameters for the parameter sets $J_\perp/J_\parallel = -0.2$, $\theta = 8\pi/9$ (blue) and $J_\perp/J_\parallel = -0.3$, $\theta = \pi$ (red). The data for $\mathcal{O}_H$ are fitted to the form: $\mathcal{O}_H \propto L^{-\alpha} \exp(-L/\xi)$.

We are grateful to K. Beach, K. Kikoin, P. Pujol, and S. Kehrein for numerous fruitful discussions. We are thankful to F. Essler for providing us additional details regarding Ref. [22]. The continuous time QMC simulations were performed using the looper code [16] (see http://wistaria.comp-phys.org/alps-looper) from the ALPS libraries [29] (see http://alps.comp-phys.org). We thank IDRIS (Orsay), CALMIP (Toulouse), and LRZ-Münich for use of supercomputer facilities. C. B. acknowledges financial support from the DFG under the Grant No. AS120/4-2. S. C. and F. A. are supported by the French ANR program. M. N. K. appreciates support from the Heisenberg program of the DFG and the SFB-410 research grant and acknowledges support from US DOE, Office of Science, under Contract No. DE-AC02-06CH11357. D. N. A. thanks ICTP for the hospitality. S. C. and F. F. A. benefit from a European exchange program (Procope).

*On leave from Petersburg Nuclear Physics Institute, Gatchina 188300, Russia.

[1] E. Dagotto and T. M. Rice, Science **271**, 618 (1996).
[2] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[3] I. Affleck and E. H. Lieb, Lett. Math. Phys. **12**, 57 (1986).
[4] A. O. Gogolin, A. A. Nersesyan, and A. M. Tsvelik, *Bosonization and Strongly Correlated Systems* (Cambridge University Press, Cambridge, England, 1998).
[5] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).
[6] D. G. Shelton, A. A. Nersesyan, and A. M. Tsvelik, Phys. Rev. B **53**, 8521 (1996).
[7] S. Larochelle and M. Greven, Phys. Rev. B **69**, 092408 (2004).
[8] H. Suhl, Phys. Rev. **109**, 606 (1958); T. Nakamura, Prog. Theor. Phys. **20**, 542 (1958); D. N. Aristov *et al.*, Z. Phys. B **95**, 291 (1994).
[9] Although there is no Kondo physics involved in the model (1), we preserve the historical name "Kondo necklace" given by Doniach [10].
[10] S. Doniach, Physica (Amsterdam) **91B**, 231 (1977).
[11] M. N. Kiselev, D. N. Aristov, and K. Kikoin, Phys. Rev. B **71**, 092404 (2005).
[12] M. N. Kiselev, D. N. Aristov, and K. Kikoin, Physica (Amsterdam) **359–361B**, 1406 (2005).
[13] D. N. Aristov, M. N. Kiselev, and K. Kikoin, Phys. Rev. B **75**, 224405 (2007).
[14] Y. Hosokoshi *et al.*, Phys. Rev. B **60**, 12 924 (1999).
[15] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983); Phys. Lett. **93A**, 464 (1983).
[16] S. Todo and K. Kato, Phys. Rev. Lett. **87**, 047203 (2001).
[17] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
[18] This hidden order is at best understood by starting with an $S = 1$ Néel state and disordering it by adding an arbitrary number of sites with $S^z = 0$ between each spin.
[19] M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989).
[20] F. Anfuso and A. Rosch, Phys. Rev. B **75**, 144420 (2007).
[21] C. Brünger *et al.* (to be published).
[22] F. H. L. Essler, T. Kuzmenko, and I. A. Zaliznyak, Phys. Rev. B **76**, 115108 (2007).
[23] H. G. Evertz, Adv. Phys. **52**, 1 (2003).
[24] A. Sandvik, Phys. Rev. B **57**, 10 287 (1998).
[25] K. S. D. Beach, arXiv:cond-mat/0403055.
[26] We note that when increasing the twist for $\theta = 0$ to $\theta = \pi/2$ at values of $|J_\perp|/J_\parallel < 1$ the spin gap grows (see Fig. 2). This could be consistent with logarithmic corrections to the gap which depend on the twist. It is beyond the scope of this numerical study to confirm this.
[27] By use of the fermionic theory [11], an estimate for the critical angle $\pi - \theta_c \sim |J_\perp/J_\parallel|$ can be found for the case $|J_\perp| \ll J_\parallel$ as the angle corresponding to a diverging mass at the Γ point of the 1D Brillouin zone. For $\theta > \theta_c$, the spectrum curvature is negative while for $\theta < \theta_c$ it is positive. Therefore, the corresponding critical exchange coupling along the second leg $J_\parallel \cos^2(\theta_c/2)$ scales as $J_\perp^2/J_\parallel$. The details of the analysis will be given elsewhere [21].
[28] Long range interaction along the second leg is referred as RKKY (Ruderman-Kittel-Kasuya-Yosida) interaction in Ref. [22]. Reserving the notation of RKKY for the models of itinerant electrons mediating the spin-spin interaction, we use the terminology of Suhl-Nakamura interaction for the models of interacting local spins as more appropriate.
[29] F. Alet *et al.*, J. Phys. Soc. Jap. Suppl. **74**, 30 (2005); M. Troyer, B. Ammon, and E. Heeb, Lect. Notes Comput. Sci. **1505**, 191 (1998).