Spin gap and string order parameter in the ferromagnetic Spiral Staircase Heisenberg Ladder: a quantum Monte Carlo study

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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 characterising 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.

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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 paper, we will focus on the opening of the spin gap for the case of two inequivalent chains coupled with a ferromagnetic rung coupling $J_\perp < 0$. This model is dubbed the Spiral Staircase Heisenberg Ladder:

$$\begin{aligned}\hat{H} &= J_\parallel \sum_i \left(\hat{\mathbf{S}}_{1,i} \cdot \hat{\mathbf{S}}_{1,i+1} + \cos^2(\theta/2)\, \hat{\mathbf{S}}_{2,i} \cdot \hat{\mathbf{S}}_{2,i+1}\right) \\ &+ J_\perp \sum_i \hat{\mathbf{S}}_{1,i} \cdot \hat{\mathbf{S}}_{2,i}. \end{aligned} \quad (1)$$

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. 1a) with twist performed along one of the legs. Such a spiral structure is characterized by the angle θ (see Fig. 1b) and interpolates between the isotropic ladder ($\theta = 0$) and a ferromagnetic SU(2) Kondo Necklace [8] model ($\theta = \pi$) [9, 10, 11, 12]. A motivation to study this specific geometry comes from the fact that a realization of the model schematically presented in Fig. 1c was synthesized as a stable organic biradical crystal PNNNO [13]. Possible candidates for realizations with twist angle $0 < \theta < \pi$ might be found in the families of molecular chains decorated by magnetic radicals.

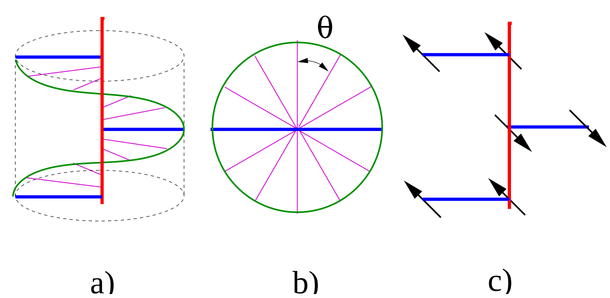

FIG. 1: (Color online) (a) Sketch of Spiral Staircase Heisenberg Ladder. (b) View of the model from the top. (c) For $\theta = \pi$, the model maps to the 1D SU(2) ferromagnetic Kondo necklace model [8].

In the strong coupling limit, $|J_\perp/J_\parallel| \gg 1$, the model

*On leave from Petersburg Nuclear Physics Institute, Gatchina 188300, Russia maps onto the spin-1 Heisenberg chain with effective exchange interaction $J_{\text{eff}} = \frac{J_\parallel}{4}\left(1+\cos^2(\theta/2)\right)$. This phase has a spin gap [14] given by $\Delta_H/J_{\text{eff}} = 0.41048(6)$ [15] and is characterized by a non-local string order parameter [16] (see a recent discussion in [17]):

$$\langle \hat{\mathcal{O}}_s(n)\rangle = \langle \hat{S}^z_{n_0} \exp\left[i\pi \sum_{j=n_0}^{n_0+n} \hat{S}^z_j \right] \hat{S}^z_{1,n+n_0}\rangle \qquad (2)$$

with $\hat{S}^z_j = \hat{S}^z_{1,j} + \hat{S}^z_{2,j}$. The expectation value picks up the hidden antiferromagnetic ordering. 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 $\theta=\pi$ [18]. A flow equation calculation has recently been carried out for the $SU(2)$ Kondo necklace model [19], (i.e. $\theta = \pi$ in Eq. (1)) and predicts a finite critical value of $J_\perp$ below which the spin gap is absent. To disentangle this situation, we have performed large scale quantum Monte Carlo (QMC) simulations of the ferromagnetic spiral staircase model. Two variants of the loop algorithm [20] 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 [21, 22]. 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 [15].

Our results for the spin gap in units of J_{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_{eff}, next to invariant thereby showing that a *small* twist is an irrelevant perturbation [23]. 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. 2b). Here and in what follows, we neglect logarithmic corrections in our discussion. Fig. 2b 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 [24], the data allows 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 $J_\perp$ as predicted in Ref. 19. 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 [18], we instead assume the existence of an inflection point and fit the data to a quadratic form

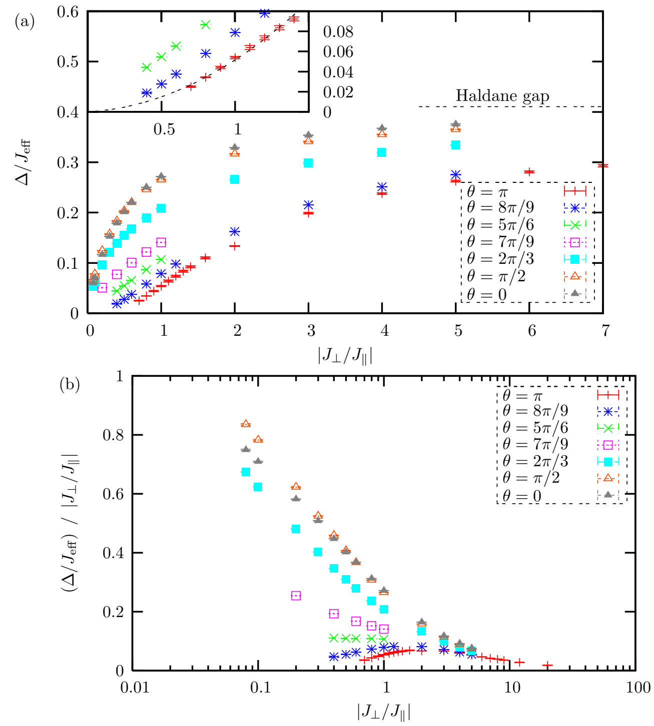

FIG. 2: (Color online) (a) Spin gap $\Delta(J_\perp)$ as a function of $|J_\perp/J_\parallel|$ for different twist angles θ. The gap is rescaled by $J_{\text{eff}} = \frac{J_\parallel}{4}\left(1+\cos^2(\theta/2)\right)$ such that in the large-$|J_\perp|$-limit, it converges asymptotically toward the 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 semi-logarithmic scale.

in the limit $J_\perp \to 0$ (see inset of Fig. 2a). 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 quicker). Indeed, such as 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) [25] interaction [26]. In second order perturbation theory, without attempting any self-consistent calculation, this interaction takes the form in $J_{SN}(q) \propto J_\perp^2 \chi_s(q,\omega=0)$ 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 treatment is to allow for a gap, Δ, in

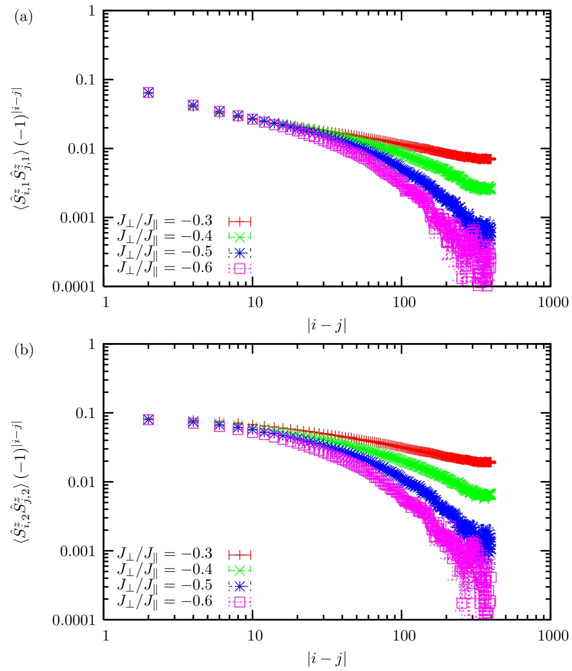

FIG. 3: (Color online) Spin-spin correlation function on both legs for the Kondo necklace model ($\theta = \pi$) at different couplings $J_\perp/J_\parallel$ on a 2×800 lattice. Simulations are carried out at $\beta J_\parallel = 7000$ ($J_\perp/J_\parallel = -0.3, -0.4$), $\beta J_\parallel = 5000$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

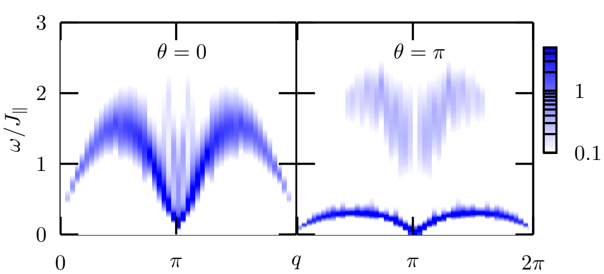

FIG. 4: (Color online) Dynamical spin-spin correlations at $J_\perp/J_\parallel = 1$ for the ladder system ($\theta = 0$) and the Kondo necklace model ($\theta = \pi$). Here we consider a bonding combination of the spins across the rungs. ($\beta J_\parallel = 200$, $L = 100$)

$\chi_s(q, \omega = 0)$. 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 spins degrees of freedom on the second leg. Due to 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 apparent, a narrow magnon band emerges as the an-

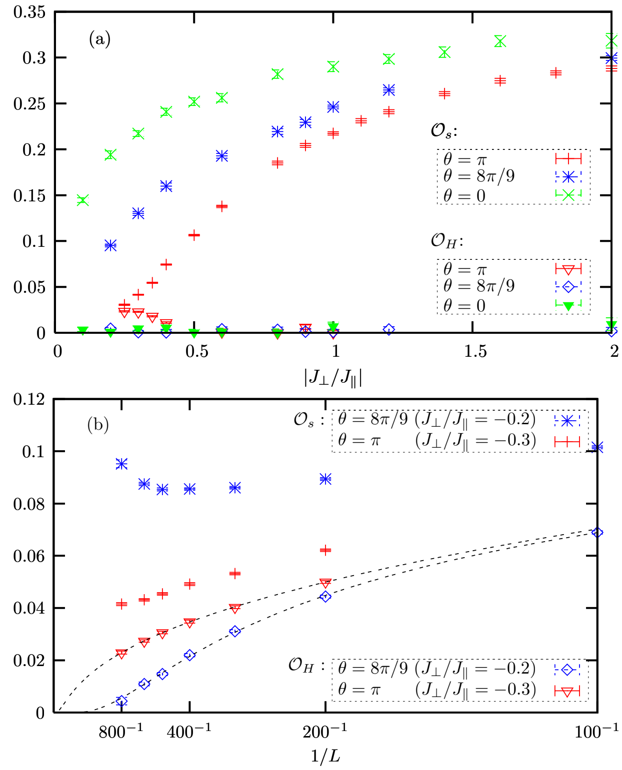

FIG. 5: (Color online) (a) String order parameter $\mathcal{O}_s$ and $\mathcal{O}_H$ as a function coupling $J_\perp/J_\parallel$ and several twist angles. For $\theta = 8\pi/9, \pi$ finite size effects are still present for the considered $L = 800$ lattice in the parameter range $|J_\perp/J_\parallel| < 0.5$. 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: $\mathcal{O}_H \propto L^{-\alpha}\exp(-L/\xi)$.

gle 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 $J_{SN} \propto J_\perp^2/J_\parallel$.

The above arguments and data suggest that irrespective of the twist angle and coupling $J_\perp$, the ground state of the model corresponds to a 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. 5a), which is finite in the Haldane phase [16]. Strictly speaking, this is not a sufficient condition to ascertain the Haldane physics since we also need to show that $\mathcal{O}_H = \langle \exp\left[i\pi\sum_{j=n_0}^{n_0+n}\hat{S}^z_j\right]\rangle|_{n=L/2}$ vanishes in the thermodynamic limit (when both $\mathcal{O}_s > 0$ and $\mathcal{O}_H > 0$, an Ising order is present [16]).

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 non-zero 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. 5b 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 a Haldane system, 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 quicker 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 $J_\perp^2/J_\parallel$.

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[24] By use of the fermionic theory [10], 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 [18].
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