Spin-Peierls instability in the three-leg Heisenberg ladder

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Because the three-leg ladder behaves like a renormalized single Heisenberg chain we argue that a spin-Peierls instability must occur in this system when it is coupled to three-dimensional phonons. Using the bond-mean-field theory, we show that this is indeed the case. The dimerized state below the spin-Peierls transition temperature forms into the columnar dimerized phase not the staggered one. This contrasts with the argument based on antiferromagnetism. A physical argument based rather on spin bonding into singlets explains why the columnar configuration is favored. No quantum criticality (gaplessness) can occur in the columnar arrangement of the dimerized chains.

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Interest in the Heisenberg ladders stems from one of their most intriguing aspects: namely, the critical properties are dependent on the number of legs, and also from the various (or at least potential) exotic quantum states that can be realized in them (for a review see Refs. [1, 2]). The spin excitations in the n-leg ladders with an even number n of legs are gapped, while those with an odd n have gapless excitation spectra [1]. The even-n-leg ladders provide an example of spin liquids. The latter, defined (loosely) as gapped phases without long-ranged order (LRO), are, in particular, believed to be relevant to the physics of high-Tc superconductivity [3].

In this Letter we study the effect of phonons on the three-leg ladder. Having an odd number of legs, this system is gapless in the absence of coupling to phonons. This was confirmed, e.g., by the Monte Carlo simulations [4, 5]. In the limit of strong rung coupling the three-leg ladder behaves as an effective (renormalized) Heisenberg chain [1]. A recent thorough theoretical study on this system corroborated this point [6]. Experiments on the real three-leg ladder compound Sr$_2$Cu$_2$O$_5$ find its spin susceptibility similar to that of a (gapless) Heisenberg chain [7].

We use the Jordan-Wigner (JW) transformation [15] and bond mean-field theory (BMFT) [11, 12, 17] to show that indeed a SP transition takes place in the three-leg ladder when it is coupled to three-dimensional phonons. To the best of our knowledge, there are no other theoretical studies of this problem, and real three-leg ladders with an SP instability do not exist yet. There are, however, studies of the *intrinsically dimerized* ladders. According to Refs. [18, 19], for the antiferromagnetic three-leg ladder with dimerization preset in the staggered pattern (cf. Fig. 1i)), there exist a critical line in the dimerization-rung-coupling plane ($\delta$, $J_\perp$), where the system is gapless. Dimerized ladders provide a counterintuitive example of "restored quantum criticality", when a system (ladder) built from gapped blocks (dimerized chains) can be gapless, contrary to naive expectations. See Refs. [18, 19] and Refs. therein for more detail. Our analysis shows that this interesting phenomenon does not occur in the coupled spin-phonon ladder: when the ladder is allowed to choose the dimerization pattern from the minimum energy condition, it orders into the columnar phase (cf. Fig. 1d). In the latter case, the ladder of dimerized chains is always gapped [20]. So, the SP transition in a three-leg ladder qualitatively resembles that in a single chain.

The spin Hamiltonian for the three-leg ladder with antiferromagnetic couplings and coupled to phonons is

$$H_{3L} = \sum_{i=1}^{N} \left[ \sum_{j=1}^{3} J_{i,i+1}(j) S_{i,j} \cdot S_{i+1,j} + J_\perp \sum_{j=1}^{2} S_{i,j} \cdot S_{i,j+1} \right],$$

(1)

where $i$ is the site label along the chains (i.e., rungs), $j = 1, 2, 3$ labels the legs (chains), and $N$ is the number of sites in a single chain; the total number of spins is $N_t = 3N$. $J_\perp$ is the coupling along the rungs and $J_{i,i+1}(j)$ is the longitudinal position-dependent coupling because the chains of the ladder are linearly coupled to the phonon field $u_{i,i+1}(j)$ [2]. Restricting our analysis to the static alternating lattice deformations $u$ along the chains, we take

$$J_{i,i+1}(j) = J_0 (1 + \gamma \langle u_{i,i+1}(j) \rangle), \quad \langle u_{i,i+1}(j) \rangle \propto (-1)^i u.$$

(2)

In this (adiabatic) approximation the phonon Hamiltonian is given by its static deformation part

$$H_{ph} = \frac{1}{2} N_t K u^2 = \frac{1}{2} \frac{N_t J_0 \delta^2}{\lambda},$$

(3)

where the dimensionless dimerization parameter $\delta \equiv \gamma u$ and the spin-phonon coupling $\lambda \equiv J_0 \gamma^2/K$. The alter-
nated frozen intrachain displacements [2] result in dimerization of each of the three chains. The dimerization of the whole ladder can be in the staggered or columnar patterns, as shown in Fig. [1].

The total Hamiltonian assumes then the form
\[ H = H_{3L} + H_{ph}, \]
and the effective intrachain spin coupling dependent on the dimerization pattern is
\[ J_{ij+1}(j) = J_0[1 + (-1)^i\delta] \quad \text{staggered} \quad (4) \]
\[ J_{ij+1}(j) = J_0[1 + (-1)^i\delta] \quad \text{columnar} \quad (5) \]

The BMFT we apply to the JW fermions consists of two key approximations. First, in dealing with the phases resulting from the JW transformation, the phase differences due to hopping of the JW fermions around any given elementary plaquette is set to be equal to \( \pi \). Second, the quartic JW fermionic terms \( c_i^{\dagger} c_i c_{i+1}^{\dagger} c_{i+1} \) resulting from the Ising interactions are decoupled using the bond parameters [6, 11, 15, 16, 17]. The latter are defined as \( Q_+ = \langle c_{2i,j} c_{2i+1,j}^{\dagger} \rangle \), \( Q_- = \langle c_{2i+1,j} c_{2i,j}^{\dagger} \rangle \) for \( j = 1, 3 \); and \( Q'_+ = \langle c_{2i,j} c_{2i+2,j}^{\dagger} \rangle \), \( Q'_- = \langle c_{2i+2,j} c_{2i,j}^{\dagger} \rangle \) for \( j = 2 \). For chains 1 and 3, the same bond parameters are used because the ladder is symmetric under exchanging chain labels 1 and 3 [6]. In the direction along the rungs, only one bond parameter is sufficient, \( P = \langle c_{2i,j} c_{2i,j+1}^{\dagger} \rangle \). For the reasons to be explained below, we will concentrate on the columnar dimerization pattern [6]. Fourier transforming along the chains direction, keeping the chains labels because of the open boundary conditions along the rungs, and using the Nambu formalism, the BMFT yields the single-particle effective Hamiltonian
\[ H^{(co)} = \sum_k \Psi_k^{\dagger} \mathcal{H}^{(co)} \Psi_k + C_t, \]
where the Hamiltonian density \( \mathcal{H}^{(co)} \) is a \( 6 \times 6 \) matrix given by
\[ \mathcal{H}^{(co)} = \begin{pmatrix} 0 & A & 0 & 0 & 0 & 0 \\ 0 & 0 & C & 0 & 0 & 0 \\ 0 & 0 & 0 & A^* & 0 & 0 \\ 0 & 0 & 0 & 0 & C & 0 \\ 0 & 0 & 0 & 0 & 0 & A \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \]
and the Nambu spinor \( \Psi_k^{\dagger} = \begin{pmatrix} c_{ik}^{\dagger} & c_{i-1,k}^{\dagger} & c_{i,k}^{\dagger} & c_{i-1,k}^{\dagger} & c_{i,k}^{\dagger} & c_{i-1,k}^{\dagger} \end{pmatrix} \). Here \( c_{ik}^{\dagger} \) is the Fourier transform of \( c_i^{\dagger} \) along the chain \( j \); i.e., with respect to the index \( i \) (\( \alpha = A \), or \( B \)), and because of the antiferromagnetic correlations the lattice is subdivided into two sublattices \( A \) and \( B \). The parameters entering the effective Hamiltonian are:
\[ A^t = (J_{1t}^t e^{ik} - J_{1t}^t e^{-ik})/2, \]
and
\[ C = J_{11}/2, \]
where
\[ J_{1t}^{\pm} = J_0(1 \pm \delta)(1 + 2Q_{\pm}^t), \]
\[ J_{11} = J_1(1 + 2P), \]
\[ C_t = N J_t |Q_+|^2 + N J_t |Q_-|^2 + \frac{3N J_0^2}{2\lambda}. \]
Here, \( J_{1t}^{\pm} = J_{1t}^{\pm} \) for \( Q_{\pm}^{t} = Q \) or \( J_{1t}^{\pm} \) for \( Q_{\pm}^{t} = Q' \). Diagonalizing \( \mathcal{H}^{(co)} \) yields six energy eigenvalues \( \pm E_j^{(co)}(k) \), \( j = 1, 2, 3 \), where
\[ E_1^{(co)}(k) = \frac{1}{2} \sqrt{\lambda}, \]
and
\[ E_2^{(co)}(k) = \frac{1}{2} \sqrt{(z - z')^2 + 8J_1^2(z + z') + 16J_{11}^2} = \frac{1}{2} \sqrt{(z - z')^2 + 8J_1^2(z + z') + 16J_{11}^2}, \quad n = 2, 3. \]

In Eqs. [9,10] \( z = (J_{1t}^t)^2 + (J_{1t}^-)^2 - 2J_{1t}^t J_{1t}^- \cos(2k), \)
\[ t = (J_{1t}^- J_{1t} + J_{1t}^- J_{1t}^-) \cos(2k) - (J_{1t} J_{1t} + J_{1t} J_{1t}^-). \]
In the absence of dimerization \( \delta = 0 \), the energy eigenvalues [9,10] coincide with those found in Ref. [6].

The partition function of the single-particle Hamiltonian [6] can be calculated and leads to the following free energy per spin
\[ F^{(co)} = \frac{C_t}{3N} - \frac{1}{2\beta N} \sum_{p=\pm} \sum_k \sum_{j=1}^3 \ln[1 + e^{\beta E_j^{(co)}(k)}], \]
where \( \beta = 1/k_B T \). Finally, the mean-field equations are derived from minimization of the free energy [11] with
FIG. 2: The free energies of the three-leg ladder without phonons ($\lambda = 0$, no dimerization), and in the presence of phonons ($\lambda = 0.1$) for the staggered and columnar configurations are plotted as functions of temperature.

respect to the six mean-field parameters $Q_\pm, Q'_\pm, P$ and $\delta$. These self-consistent (integral) equations are solved numerically.

The mean-field equations predict no magnetic long range order (LRO), even at zero temperature. At the same time, they predict the simultaneous appearance at some critical temperature of the structural LRO (lattice dimerization $\delta$) and the spin gap, generated by $\delta \neq 0$. So, this is a SP transition.

First, we compare the free energies of the two dimerization patterns. For the staggered configuration with the effective coupling $\hat{H}$, the single-particle effective Hamiltonian, its spectrum, and the mean-field equations are derived in the same manner as described above for the columnar configuration. Fig. 2 shows the free energies as functions of temperature for both dimerized configurations and without dimerization ($\lambda = 0$). The free energy of the dimerized columnar configuration is lower than those of the staggered or non-dimerized configurations below a nonzero temperature, which we identify as the SP temperature $T_{SP}$. So, the columnar order constitutes the thermodynamically stable state at low temperature. Above $T_{SP}$ the dimerization disappears, and all three free energies become equal. We also plot $\frac{\Delta F}{|F(\alpha)|} = \frac{F(\alpha) - F(\alpha^*)}{|F(\alpha)|}$ as a function of $\alpha \equiv J_\perp/J_0$ at practically zero temperature in Fig. 3 for $\lambda = 0.5$. $\frac{\Delta F}{|F(\alpha)|}$ increases as $\alpha$ increases passes through a maximum, then decreases rapidly in the strong coupling regime $\alpha \gg 1$. This means that the staggered and columnar states become practically degenerate when $\alpha \gg 1$.

To understand why the columnar configuration is the stable one, assume $\alpha$ is large. In this limit, the three-leg ladder behaves pretty well like a single Heisenberg chain with an effective coupling, and the spin degrees of freedom on two of the chains freeze into spin singlets on the rungs $\hat{H}$. It is then favorable for the coupling along the chains to couple the singlets into a plaquette (which gives rise to a linear combination of transverse and longitudinal spin singlets for the spins on four of the six sites) like in Fig. 1(b). The staggered configuration would be favorable if the spins on the rungs were ordered antiferromagnetically. For intermediate and weak values of the rung coupling $\alpha$, the spins are not frozen but are nonetheless locked into random singlets on two of the three chains $\hat{H}$, and the argument based on spins singlets still holds, while that based on antiferromagnetically ordered spins on the rungs continues to be wrong.

The mean-field parameters are plotted as functions of temperature in Fig. 4 for $\lambda = 1$ and $\lambda = 1$. At $T_{SP}$, a spin gap opens and a structural phase transition occurs from the disordered phase into the dimerized phase. This is clearly indicated by the temperature dependence of $\delta$ in the inset of figure 4(b), which is very similar to that in an ordinary second-order phase transition. The other (bond) parameters are not critical. Below $T_{SP}$, $Q^\perp_+ \neq Q^\perp_-$ due to non-zero dimerization, while $Q^\perp_? = Q^\perp_?$ above $T_{SP}$.

The SP instability is accompanied by the opening of an energy gap in the spin excitation spectra (spin gap). The spin excitation energies consist of three bands $E_j(k)$, Eqs. (10), with $E_2$ and $E_3$ gapped even in the absence of dimerization with a gap of the order of $J_\perp$. The gap in $E_1(k)$ is induced by the dimerization $\delta$. We plot $E_1(k)$ for the columnar dimerized ($\lambda = 0.7$) and non-dimerized ($\lambda = 0$) ladder in Fig. 5. The spectrum of the non-dimerized three-leg ladder, calculated in Ref. 6 is gapless, i.e., $E_1(0/\pi) = 0$, as it should be for an odd-leg ladder $\hat{H}$. (Note the symmetry of $E_j(k)$ with respect to the point $k = \frac{\pi}{2}$.) The spin gap $E_g = E_1(0)$ defined from

FIG. 3: The free energy difference between the staggered and columnar configurations as a function of $\alpha \equiv J_\perp/J_0$ at $T = 0.009 J_0$, $\lambda = 0.5$.

FIG. 4: The temperature dependence of the mean-field parameters $Q_\pm, Q'_\pm, P$ and $\delta$ for $\alpha = 1, \lambda = 1$.
Eqs. (8) and (9) is

$$E_g = J_0 \delta(1 + \lambda_{\perp} + \lambda_{\parallel}) + (\lambda_{\perp} - \lambda_{\parallel}).$$  

(12)

So, to leading order our theory, as any mean-field one [21] gives the non-interacting fermion (equivalently, the dimerized single XY-chain) result $E_g \propto \delta$, albeit renormalized by the bond parameters $Q_{\pm}$. This is confirmed by direct numerical calculations of $E_g(\delta)$. Note that for a dimerized chain $E_g \propto \delta^{1/3}$ [22], corrected by the marginal logarithmic prefactor $\ln \delta$ [10, 22, 23]. The temperature dependence of the spin gap is shown in Fig. [6]. Both the numerical calculations and qualitative analyses of the mean-field equations show that $\delta$, $E_g$, and $T_{SP}$ increase monotonously with the phonon coupling constant $\lambda$. However the dependence of those parameters on $\alpha = J_\perp/J_0$ is trickier. The parameters $\delta$, $E_g$, and $T_{SP}$ initially decrease with growing $\alpha$, but then saturate as $\alpha \gtrsim 5$ as seen in Fig. [6]. The mechanism of such saturation was already discussed [1], and can be understood in the regime $\alpha \gg 1$ as due to the fact that the ladder behaves as a “renormalized” spin-$\frac{1}{2}$ chain.

In this work, the spin-Peierls instability in the three-leg ladder coupled to phonons is studied. We map the spin operators of the three-leg Heisenberg ladder onto Jordan-Wigner fermions. The resulting interaction terms are decoupled within the bond-mean-field theory. This theory yields a spin-Peierls transition into the columnar dimerized phase. Qualitatively, the three-leg dimerized ladder behaves like a single spin-Peierls chain. No gapless state can occur for such arrangement of the dimerized chains. Finally, we conjecture that the results derived here for the three-leg ladder should stay true for any $n$-leg ladder with $n = 5, 7, \ldots$

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FIG. 5: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$.

FIG. 6: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 7: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 8: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 9: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 10: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 11: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 12: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 13: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 14: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 15: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 16: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 17: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 18: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 19: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 20: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 21: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 22: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 23: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 24: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 25: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 26: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 27: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 28: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$. 

FIG. 29: The spectra for the uniform ($\lambda = 0$) and columnar dimerized ($\lambda = 0.7$) ladders are shown. Here, $\alpha = 1$. 

FIG. 30: The temperature dependence of the spin gap is shown for several values of $\alpha$, and for $\lambda = 0.1$.