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## The spin-Peierls chain revisited

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### Abstract

We extend previous analytical studies of the ground-state phase diagram of a one-dimensional Heisenberg spin chain coupled to optical phonons, which for increasing spin–lattice coupling undergoes a quantum phase transition from a gapless to a gapped phase with finite lattice dimerisation. We check the analytical results against established four-block and new two-block density matrix renormalisation group (DMRG) calculations. Different finite-size scaling behaviour of the spin excitation gaps is found in the adiabatic and anti-adiabatic regimes.

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Quantum phase transitions in low-dimensional correlated systems have attracted considerable attention over the last decades. An example is the Peierls instability in quasi-one-dimensional spin systems, i.e., the instability of a uniform spin chain towards dimerisation induced by the interaction with lattice degrees of freedom. Starting in the seventies with organic compounds [1], the interest in the Peierls instability was renewed with the discovery of a spin-Peierls (SP) transition in the inorganic compound CuGeO<sub>3</sub> in 1993 by Hase et al. [2]. The most significant feature distinguishing CuGeO<sub>3</sub> from other SP-compounds is the high frequency  $\omega$  of the involved optical phonons, which is comparable to the magnetic exchange interaction  $J$ .

As an archetypal model for this type of SP system we consider the anti-ferromagnetic Heisenberg chain coupled to harmonic Einstein oscillators,

$$H = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \omega \sum_i b_i^\dagger b_i + \bar{g} \sum_i (b_i^\dagger + b_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \mathbf{S}_i \cdot \mathbf{S}_{i-1}), \quad (1)$$

where  $\mathbf{S}_i$  denote spin- $\frac{1}{2}$  operators at lattice site  $i$ , and  $b_i^\dagger$  and  $b_i$  are phonon creation and annihilation operators, respectively. This model has been studied with a number of analytical and numerical methods, including second-order flow equations [3], the combination of Schrieffer–Wolff transformations [4] with a variational ansatz [5], as well as exact diagonalisation [5] and a four-block variant [6] of the density matrix renormalisation group (DMRG) [7,8]. All these studies agree on the main finding that for finite phonon frequency the system undergoes a transition from a phase with gapless spin excitations to a dimerised phase with massive spin excitations only for some finite value of the rescaled spin–phonon coupling  $g = \bar{g}/\omega$ .

In the anti-adiabatic limit  $\omega \rightarrow \infty$  this critical coupling is approaching zero, whereas in the adiabatic limit  $\omega \rightarrow 0$  flow equations and DMRG point towards a finite limiting value of  $g_c$ . This is equivalent to the bare critical coupling  $\bar{g}_c$  approaching zero linearly with  $\omega$ . To second order in  $g$ , the Schrieffer–Wolff approach is equivalent to the flow-equation result, but when fourth-order terms are included the critical coupling diverges for decreasing  $\omega$ . This finding, of course, casts doubts on the method and on the decoupling of spins and phonons by unitary transformations in general, especially in the adiabatic regime.

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Table 1

Expansion of the effective exchange interactions  $J_n/J$  up to order 8 in the electron–phonon coupling  $g$ 

	$g^0$	$g^2$	$g^4$	$g^6$	$g^8$
$J_0$		$-\frac{3\omega}{8}$	$\frac{9\omega}{64}$	$-\frac{7\omega}{64}$	$\frac{5\omega}{64}$
$J_1$	1	$\omega - \frac{3}{2}$	$-\frac{9\omega}{8} + \frac{59}{24}$	$\frac{205\omega}{144} - \frac{1123}{360}$	$-\frac{545\omega}{384} + \frac{118791}{35840}$
$J_2$		$\frac{\omega}{2} + \frac{3}{2}$	$\frac{\omega}{16} - \frac{25}{8}$	$-\frac{55\omega}{144} + \frac{145}{32}$	$\frac{313\omega}{512} - \frac{70573}{13440}$
$J_3$			$\frac{5\omega}{8} + \frac{2}{3}$	$-\frac{83\omega}{96} - \frac{3023}{1920}$	$\frac{1255\omega}{1536} + \frac{500191}{215040}$
$J_4$				$\frac{31\omega}{128} + \frac{937}{5760}$	$-\frac{2551\omega}{5760} - \frac{44533}{107520}$
$J_5$					$\frac{131\omega}{2560} + \frac{5297}{215040}$

Using improved spin algebra codes in this article we, therefore, reconsider the Schrieffer–Wolff approach for the model of Eq. (1). In more detail, we try to decouple spin and phonon degrees of freedoms by applying a unitary transformation  $\tilde{H} = \exp(S)H \exp(-S)$  that removes interaction terms linear in  $g$ ,

$$S = g \sum_i (b_i^\dagger - b_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \mathbf{S}_i \cdot \mathbf{S}_{i-1}). \quad (2)$$

Averaging the resulting Hamiltonian over the phonon vacuum we obtain an effective spin model with long-ranged Heisenberg interactions. Such frustrated spin chains are known to be susceptible to dimerisation, and we can use the ratio of the next-nearest-neighbour to the nearest-neighbour exchange,  $\alpha_{\text{eff}}$ , as an indicator of the phase transition, which for the frustrated spin- $\frac{1}{2}$  chain

$$H = \sum_i J(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha \mathbf{S}_i \cdot \mathbf{S}_{i+2}) \quad (3)$$

occurs at  $\alpha_c = 0.241167$  [9]. The transformed Hamiltonian  $\tilde{H}$  can be expanded in a series of iterated commutators,  $\tilde{H} = \sum_k [S, H]_k / k!$ , where  $[S, H]_{k+1} = [S, [S, H]_k]$  and  $[S, H]_0 = H$ . For orders  $k > 2$  the evaluation of these commutators rapidly becomes complicated, and is feasible only with efficient computer algebra tools. We were now able to push the limit of the expansion from order 4 to order 8. Neglecting terms with more than two interacting spins, the resulting effective spin Hamiltonian reads

$$H_{\text{eff}} = J_0 N + \sum_i \sum_{n=1}^5 J_n \mathbf{S}_i \cdot \mathbf{S}_{i+n} \quad (4)$$

with  $J_n = J \sum_{j=0}^4 c_{j,n} g^{2j}$  and the coefficients  $c_{j,n}$  collected in Table 1.

In Fig. 1 we show the phase diagram obtained from the condition  $\alpha_{\text{eff}} = J_2/J_1 = a_c$ . The resulting critical coupling  $g_c$  oscillates with increasing order in  $g$ . Here the second and fourth correspond to the known results of Refs. [3,5], respectively, but convergence is achieved only when going well beyond that.

It turns out, however, that the lowest-order result shows the best agreement with the four-block DMRG data of Bursill et al. [8]. On the one hand, this may not seem surprising, since the concept of integrating out phonon degrees of freedom usually is appropriate only in the anti-adiabatic limit. On the other hand, the smallest energy

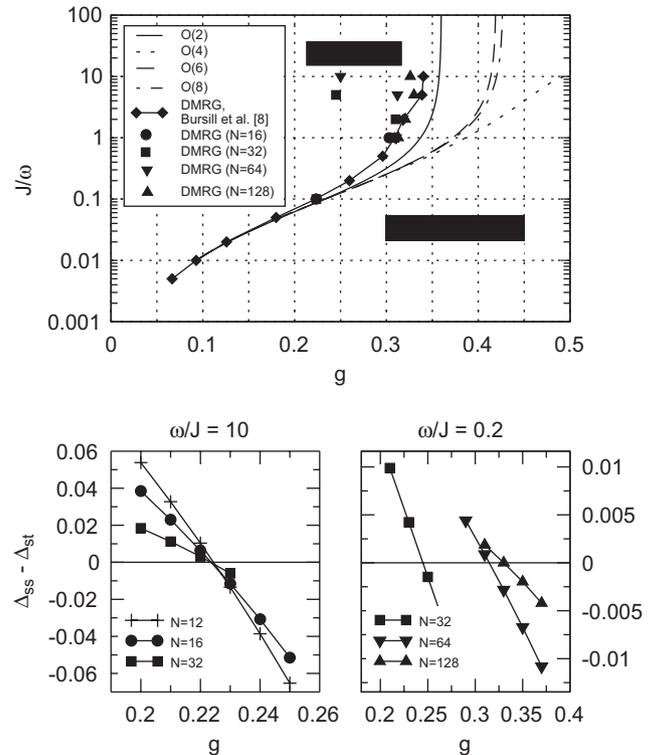


Fig. 1. Upper panel: ground-state phase diagram of the SP model, Eq. (1). Lower panel: system size dependence of the level crossing at  $g_c$  in the adiabatic and anti-adiabatic limit.

scale in the problem always corresponds to the spin degrees of freedom, and, therefore, an effective spin model should be able to describe the phase transition.

Numerically, the value of  $g_c$  is obtained from the level crossing of the lowest singlet and triplet excitations of the full spin–phonon model, Eq. (1), i.e., from the same criterion applied to get  $\alpha_c$  of the frustrated spin chain, Eq. (3). In the adiabatic limit this procedure is rather delicate, since the appropriate (finite-size) gaps must be smaller than  $\omega$ , requiring large system sizes. In addition,  $g_c$  has a noticeable system size dependence, which is negligible in the anti-adiabatic case (see lower panels of Fig. 1). To cross-check this numerical data we performed new, large-scale parallel DMRG calculations [10] using the standard lattice growth method of two sites per iteration. For comparable lattice sizes we find very good agreement.

How the unitary transformation scheme can be modified to yield improved effective Hamiltonians for the low energy physics of SP systems will be the subject of future studies.

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