The spin-Peierls chain revisited

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Abstract

We extend previous perturbative analytical studies of the ground-state phase diagram of a one-dimensional Heisenberg spin chain coupled to optical phonons via local and differential couplings, respectively. With increasing spin-lattice coupling the system undergoes a quantum phase transition from a gapless (spin liquid) to a gapped phase with finite lattice dimerisation. For the local coupling we present new perturbative analytical and large-scale density matrix renormalization group (DMRG) calculations and find deviations from previous quantum Monte Carlo and flow equation results. For the differential coupling we compare established four-block and new two-block DMRG results with a refinement of previous analytical studies.
In both cases, the spin excitation gaps show different finite-size scaling behavior in the adiabatic and anti-adiabatic regimes.

Spin-Peierls Instability

Coupling of electronic and lattice degrees of freedom leads to interesting physics already in one dimension:

- Peierls instability of 1D metals towards lattice distortions
- Mott to Peierls insulator transition in the 1D Holstein-Hubbard model
- Spin-Peierls instability in spin chains with magnetoelastic coupling

Physical examples for the latter were found in quasi-1D organic materials (TTF/TCNQ) as well as in the inorganic compound $CuGeO_3$ [1] that forms well-separated spin-1/2 chains:

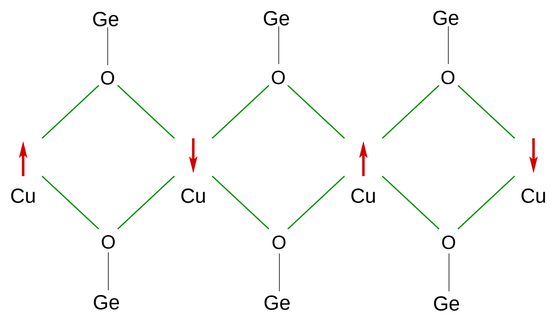

Fig. 1: *A CuO_2 chain in Copper Germanate*

Within the CuO_2 chains, neighboring spins interact via high-ω optical phonons ($\omega \approx J$) $\Rightarrow$ non-adiabatic modeling required.

Microscopic Models

Microscopic models comprise a Heisenberg spin-1/2 chain and a set of Einstein oscillators, coupled by an interaction term:

$$H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \omega \sum_i b_i^\dagger b_i + H_{sp}\,, \qquad (1)$$

with common choices for the coupling:

$$H_{sp}^{\text{diff}} = g\omega \sum_i (b_i^\dagger + b_i)(\vec{S}_i \cdot \vec{S}_{i+1} - \vec{S}_{i-1} \cdot \vec{S}_i) \qquad (2)$$

and, respectively,

$$H_{sp}^{\text{loc}} = g\omega \sum_i (b_i^\dagger + b_i)\vec{S}_i \cdot \vec{S}_{i+1}\,. \qquad (3)$$

All analytical and numerical approaches so far agree on the following scenario:

weak coupling	spin liquid, gapless
strong coupling	lattice dimerization, massive spin excitations

The basic mechanism of the phase transition is well understood — effective spin interactions beyond next-neighbor exchange lead to effective frustrated models, which are known to be susceptible to dimerization beyond some critical frustration.
Example: In the frustrated Heisenberg spin chain

$$H = \sum_i (\vec{S}_i \cdot \vec{S}_{i+1} + \alpha \vec{S}_i \cdot \vec{S}_{i+2})\,, \qquad (4)$$

dimerization sets in at $\alpha_c = 0.241167$ [2].

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[2] S. Eggert, Phys. Rev. B **54**, R9612 (1996).

Schrieffer-Wolff Transformation

Analytical approach: Unitary transformation eliminates spin-phonon interactions to leading order:

$$\tilde{H} = \mathrm{e}^S H \mathrm{e}^{-S}\,, \qquad (5)$$

with S chosen appropriately, e.g.,

$$S^{\text{diff}} = g \sum_i (b_i^\dagger - b_i)(\vec{S}_i \cdot \vec{S}_{i+1} - \vec{S}_i \cdot \vec{S}_{i-1}) \qquad (6)$$

for the difference coupling and

$$S^{\text{loc}} = g \sum_i (b_i^\dagger - b_i)\vec{S}_i \cdot \vec{S}_{i+1} \qquad (7)$$

for local coupling. $\tilde{H}$ can only be expressed in a series expansion

$$\tilde{H} = \sum_k \frac{[S,H]_k}{k!}\,, \text{ with } [S,H]_{k+1} = [S,[S,H]_k] \qquad (8)$$

and $[S,H]_0 = H$. The terms must be evaluated using computer algebra tools (FORM [8]).
Subsequently, averaging over the phonon vacuum or, more generally, over coherent states $|\xi\rangle$ with $b_i|\xi\rangle = \xi|\xi\rangle$, yields an effective spin-only Hamiltonian

$$\begin{aligned} H_{\text{eff}} &= \langle\xi|\tilde{H}|\xi\rangle \\ &= J_0 N + \sum_i \sum_{n=1}^{n_{\max}} J_n \vec{S}_i \cdot \vec{S}_{i+n} + H_{\text{ms}}\,, \end{aligned} \qquad (9)$$

with $J_n = J \sum_{j=0}^{j_{\max}} c_{j,n}\, g^{2j}$. All terms with more than two interacting spins are collected in H_{ms} and neglected hereafter.
The phase boundary is then fixed by the condition

$$\alpha_{\text{eff}} = \frac{J_2}{J_1} \stackrel{!}{=} \alpha_c\,, \qquad (10)$$

where α_c is known from the frustrated Heisenberg spin chain (4).

DMRG

Numerical approach: DMRG is well-suited for the study of 1D spin-phonon systems. DMRG provides an algorithm that can iteratively select an "optimal" set of basis states in order to describe observables. The number of density matrix states kept, m, determines the cutoff error, or "discarded weight" W_m. For $m \to \infty$, DMRG becomes exact. We use a high-performance DMRG code that

- utilizes pseudo-bosons to model a Hilbert space with 2^n real phonons using just n pseudo-bosons with appropriate commutation rules
- is shared-memory parallelized (using OpenMP) in the most important region, i.e. the diagonalization of the superblock Hamiltonian

DMRG calculations for this work were carried out with m up to 1000. As the cutoff error in low-lying energy levels from the exact values is $\propto W_m$, extrapolation of gaps towards $m \to \infty$ is simple and was always performed.

Detection of the phase transition is done by an established level-crossing criterion,

$$\Delta_{\text{ss}}(g_c) = \Delta_{\text{st}}(g_c)\,, \qquad (11)$$

where Δ_{ss} and Δ_{st} are the singlet and triplet excitation gaps, respectively. The gaps behave as follows:

	$N < \infty$	$N \to \infty$
$g < g_c$	$\Delta_{\text{ss}} > \Delta_{\text{st}}$	$\Delta_{\text{ss}} = \Delta_{\text{st}} = 0$
$g > g_c$	$\Delta_{\text{ss}} < \Delta_{\text{st}}$	$\Delta_{\text{ss}} = 0,\ \Delta_{\text{st}} > 0$

Caveat: In the adiabatic regime ($\omega << J$) the singlet excitation is easily confused with the ground state plus one phonon. Large N is required in this limit in order to get the correct crossing criterion. In general, one needs $N \geq 128$ in the low-ω region.

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[4] K. Kuboki and H. Fukuyama, J. Phys. Soc. Jpn. **56**, 3126 (1987).
[5] A. Weiße, G. Wellein, and H. Fehske, Phys. Rev. B **60**, 6566 (1999).

Difference Coupling — Status

Studied previously using a variety of approaches:

- Second-order flow equations [3]
- Schrieffer-Wolff transformation and variational ansatz [4, 5]
- Exact diagonalization (ED) [5]
- Four-block DMRG [6]

All agree on the existence of a finite g_c marking the phase boundary between spin liquid and dimerized phase with spin gap.

$\omega \to \infty$	$g_c \to 0$
$\omega \to 0$	$g_c > 0 \Rightarrow g_c\omega \to 0$

The phase diagram had previously been established numerically by 4-block DMRG calculations, in fair agreement with 2nd order Schrieffer-Wolff approach. But: 4th order deviates significantly!

Goal: Extend perturbative Schrieffer-Wolff calculations to higher order and check against two-block parallel DMRG results.

Difference Coupling — Results [9]

The perturbative Schrieffer-Wolff approach was carried out up to order 8 in the coupling (previously 4). The Hamiltonian was averaged over the phonon vacuum ($\xi = 0$), yielding the following expansion coefficients $c_{j,n}$:

	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					$\frac{131\omega}{2560} + \frac{5297}{215040}$

Here $n_{\max} = 5$ and $j_{\max} = 4$, respectively. DMRG with the crossing criterion yields different finite-size scaling in the adiabatic and anti-adiabatic regimes. The critical coupling is more or less independent of N for large ω, but depends heavily on N for $\omega \lesssim 1$:

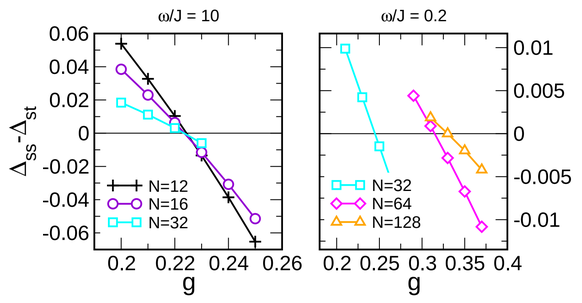

Fig. 2: *Varying dependence of level crossing criterion on N for difference coupling*

The phase diagram can now be established. Interestingly, the lowest-order perturbation result shows best agreement with the four-block DMRG data:

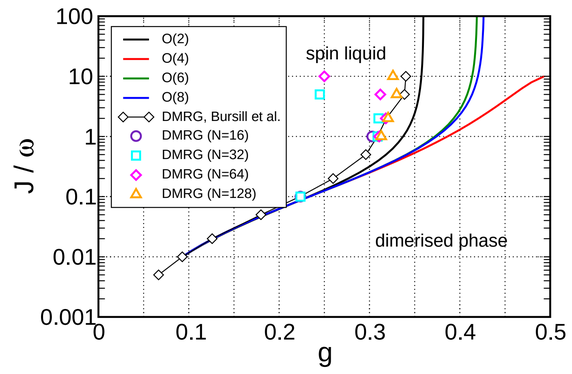

Fig. 3: *Phase diagram of magnetoelastic spin-phonon chain with difference coupling*

The two-block DMRG results refine the four-block data somewhat, but there is still a discrepancy to the $O(8)$ perturbative result in the adiabatic regime. This is, however, put into perspective by the fact that the "bare" coupling $\bar{g}_c = g_c\omega$ approaches zero linearly with ω in this limit.

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Local Coupling — Status

Local coupling applies to $CuGeO_3$. The precise location of the phase boundary is arguable according to previous studies using

- Schrieffer-Wolff approach, variational ansatz [5]
- Exact diagonalization [5]
- Flow equations [7]
- Quantum Monte Carlo (QMC) [7]

Flow equations and QMC tend to underestimate the critical coupling compared to the other methods. Generally, the phase structure is similar to the situation with difference coupling, but with a finite $g_c > 0$ in the antiadiabatic limit.

Goal: Shed light on the controversial position of the phase boundary by higher-order Schrieffer-Wolff approximations. Check against large-scale parallel DMRG results.

Local Coupling — Results [10]

The perturbative Schrieffer-Wolff analysis can be carried out to $O(12)$ in the coupling constant (inset of Fig. 5). For DMRG, again, the crossing criterion is strongly dependent on N for $\omega \lesssim 0.5$:

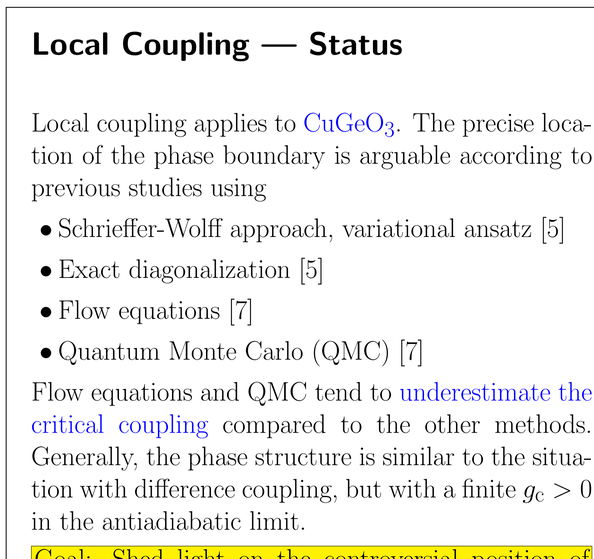

Fig. 4: *Dependence of level crossing criterion on N for local coupling*

The phase diagram shows that the qualitative behavior (slope) of the phase boundary is captured well be the highest-order perturbation result at vanishing phonon shift ($\xi = 0$). A phonon shift of $\xi \approx 0.44g/\omega$ describes the adiabatic regime of the phase boundary strikingly well, but this is just coincidence as an extrapolation of the DMRG data to the thermodynamic limit clearly shows (green triangles in Fig. 5).

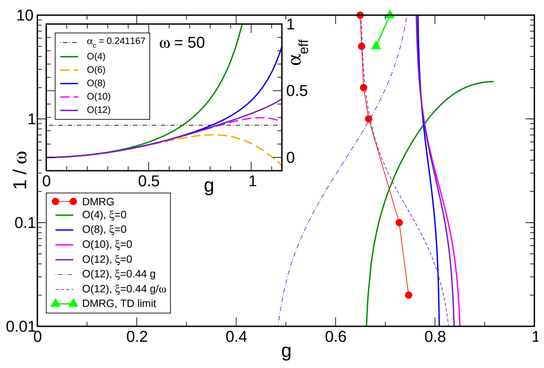

Fig. 5: *Phase diagram for local coupling*

Conclusions

Using DMRG, we obtained the to date most precise numerical result for the location of the quantum phase transition from the spin liquid to the dimerized phase in the one-dimensional Heisenberg model with local coupling and difference coupling to optical phonons. In both cases, we proved the convergence of the unitary transformation approach that maps the full spin-phonon model to an effective frustrated spin model and allows an analytical calculation of the phase boundary in good agreement with the numerical data.

Acknowledgement

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[8] J. A. M. Vermaseren, `math-ph/0010025`
[9] G. Hager, *et al.*, `cond-mat/0606360`
[10] A. Weiße, G. Hager, A. R. Bishop, and H. Fehske, `cond-mat/0607209`