Effective Spin Models for Spin-Phonon Chains by Flow Equations

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We investigate the anti-adiabatic limit of an antiferromagnetic $S=1/2$ Heisenberg chain coupled to Einstein phonons. The flow equation method is used to decouple the spin and the phonon part of the Hamiltonian. In the effective spin model long range spin-spin interactions are generated. We determine the phase transition from a gapless state to a gapped (dimerized) phase, which occurs at a non-zero value of the spin-phonon coupling. In the effective phonon sector a phonon hardening is observed.

Dedicated to Professor E. Müller-Hartmann on the occasion of his 60th birthday.

I. INTRODUCTION

The interest in the spin-Peierls (SP) transition [1] has been renewed by the discovery of the first inorganic SP substance CuGeO$_3$ [2,3]. The SP instability of quasi one-dimensional spin systems is the analogon of the Peierls instability of quasi one-dimensional metals towards lattice modulations with a wave vector $2k_F$. Due to the coupling of the lattice degrees of freedom to the $d=1$ magnetic degrees of freedom the system can lower its energy by undergoing a phase transition into a dimerized state. The loss in elastic energy is overcompensated by the gain in the magnetic energy.

Most theoretical studies of SP transitions rely on an adiabatic treatment of the phonons (e.g. Ref. [4]). This means that the energy of the phonons, that are associated with the lattice distortion, should be low compared with the spin-spin exchange coupling. In addition to the occurrence of a pre-existing soft phonon, one observes a phonon softening in the organic SP compounds. Furthermore, the phonon energy $\omega$ should be small compared with the resulting gap $\Delta$ in the spin excitation spectrum [5].

It has been recently emphasized [6], that CuGeO$_3$ does not fulfill these conditions. Even more, a phonon hardening by about 5%–6% is observed [7]. Uhrig [6] has developed a flow equation approach [8] which is not founded on adiabaticity. The comparison with the DMRG data of Bursill et al. [9] has shown that the flow equation method works well, especially in the limit of small $J/\omega$ (cf. Fig. 1 in Ref. [9]). In this paper we extend this approach. Details will be given below.

II. FLOW EQUATION APPROACH

The method of our choice is the flow equation approach introduced by Wegner [8]. This method is similar to Fröhlich’s approach [10], which projects a Hamilton operator to an effective Hamiltonian in one step applying an unitary transformation. Wegner modified the Fröhlich transformation as he uses an infinite number of infinitesimal unitary transformations.

The model we study reads

$$\mathcal{H}(\ell) = \mathcal{H}_S + \mathcal{H}_{SB} + \mathcal{H}_B$$

$$\mathcal{H}_S = \sum_i (J_1(\ell) S_i S_{i+1} + J_2(\ell) S_i S_{i+2})$$

$$\mathcal{H}_B = \sum_i \left[ \omega(\ell) b_i^\dagger b_i + \frac{\mu(\ell)}{2} (b_i^\dagger b_i^\dagger + b_i b_i) \right]$$

$$\mathcal{H}_{SB} = \sum_i (A_i(\ell) b_i^\dagger + A_i^\dagger(\ell) b_i) \ .$$

Here $S_i$ stands for the $S=1/2$ spin operator on site $i$ and $b_i$ ($b_i^\dagger$) destroys (creates) a phonon on site $i$. $\mathcal{H}_S$ is the Hamiltonian of a frustrated spin chain or $J_1$-$J_2$ model. If the frustration parameter $\alpha \equiv J_2/J_1$ exceeds a critical value of $\alpha = \alpha_c = 0.241167(5)$, then the model undergoes a quantum phase transition from a gapless state to a gapped phase [11–13]. We start with a Hamilton operator (1a) consisting of pure spin ($\mathcal{H}_S$) and phonon ($\mathcal{H}_B$) parts and a spin-phonon coupling term $\mathcal{H}_{SB}$ and use flow equations to decouple the spin-phonon system.

The continuous transformation is parameterized by a flow parameter $\ell \in [0, \infty)$. So $\mathcal{H}(\ell = 0)$ stands for the original Hamiltonian as given. We will end up with the effective Hamiltonian $\mathcal{H}(\ell = \infty)$ which is more “diagonal” in the way that the direct spin-phonon coupling has been rotated away. The infinitesimal generator $\eta(\ell)$ defines the unitary transformation via

$$\frac{d\mathcal{H}(\ell)}{d\ell} = [\eta(\ell), \mathcal{H}(\ell)] \ .$$

A choice of $\eta(\ell)$ proposed by Wegner is

$$\eta(\ell) = [\mathcal{H}_d(\ell), \mathcal{H}(\ell)] \ ,$$

where $\mathcal{H}_d(\ell)$ is the part of $\mathcal{H}(\ell)$ which is already diagonal in the basis of the particular model considered.
where $\mathcal{H}_d$ is the part of the Hamiltonian which is regarded as diagonal. By choosing $\mathcal{H}_d(\ell) \equiv \mathcal{H}_S(\ell) + \mathcal{H}_B(\ell)$ and the “off-diagonal” interaction part as $\mathcal{H}_{od}(\ell) \equiv \mathcal{H}_{SB}(\ell)$, our generator reads $\eta(\ell) = [\mathcal{H}_a, \mathcal{H}_{od}] = [\mathcal{H}_S + \mathcal{H}_B, \mathcal{H}_{SB}]$. In Chapter IV we present an alternative choice of $\eta$, while the canonical version (3) is used throughout the main part of this paper.

As initial conditions we choose

$$J_1(0) = J \quad \text{and} \quad J_2(0) = 0. \quad (4)$$

So the untransformed pure spin part is the normal Heisenberg Hamiltonian. As we will see later on, for non-zero values of the flow parameter $\ell$ long range spin-spin interactions arise. As a consequence, the next-nearest neighbour coupling constant $J_2$ in the effective spin model is finite. The phonon part $H_B = H_B^{(\omega)} + H_B^{(\mu)}$ includes a non-boson-number conserving term $H_B^{(\mu)}$. This choice is due to the fact, that the generator $\eta = [\mathcal{H}_S + H_B^{(\omega)}, \mathcal{H}_{SB}]$ would produce terms proportional to $b_i b_i^\dagger$ anyway. So for our purpose it is convenient to embed this terms in $\mathcal{H}$ and renormalize $\mu(\ell)$. Henceforth, we choose

$$\omega(0) \equiv \omega_0 = 1 \quad \text{and} \quad \mu(0) = 0 \quad (5)$$

and give all coupling constants in units of $\omega_0$.

$\mathcal{H}_{SB}$ describes the coupling between spin and phonon system. The spin-phonon coupling mainly influences neighbouring sites. Hence the coupling operator $A_i(0)$ typically consists of nearest neighbour spin products. An appropriate choice for $A_i(0)$ is the difference coupling

$$A_i(0) = g(S_i S_{i+1} - S_i S_{i-1}), \quad (6)$$

which does not contribute to the undistorted phase due to the translational invariance [6], i.e. $\langle A_i(0) \rangle$ vanishes. According to Ref. [8], $A_i$ should be normal-ordered, i.e. $A_i(0) \rightarrow A_i(0) - \langle A_i(0) \rangle$. This is guaranteed by the specific choice (6). By choosing different coupling operators, various mechanisms of how the lattice distortions influence the exchange integral $J$ can be investigated. In the case of the difference coupling, the exchange coupling directly depends on the “position” of a spin between the neighbouring ones. For CuGeO$_3$ this corresponds to changes of two neighbouring Cu–O–Cu binding angles, i.e. one of them is enlarged on expense of the other one.

Sometimes a local coupling $\mathcal{H}_{SB}^{loc} = g \sum_i S_i S_{i+1} (b_i^\dagger + b_i)$ is used in connexion with CuGeO$_3$ (see e.g. Ref. [14–16]): Single harmonic degrees of freedom directly modify the magnetic interaction. In Ref. [16] the gap due to dimerization was investigated by means of a high order perturbation expansion. A flow equation approach to this coupling type will be presented elsewhere [17].

Applying the unitary transformation, not only the coupling constant in (6) changes ($g \rightarrow a(\ell)$). Additionally longer range and multiple site interactions arise. Their $\ell$-dependent coupling constants are denoted by $b_n(\ell)$. The aim of this approach is to disentangle phonons and spins. Hence in the limit $\ell \rightarrow \infty$ the coupling operator $A_i(\ell)$ vanishes, i.e. $a(\infty) = 0$ and $b_n(\infty) = 0$.

We introduce the Liouville operator $\mathcal{L}$ for the commutation with $\mathcal{H}_S$:

$$\mathcal{L} | \mathcal{O} := [\mathcal{H}_S, \mathcal{O}].$$

In extension to Ref. [6] the Liouville operator $\mathcal{L}(\ell)$, the phonon frequencies $\omega(\ell)$ and $\mu(\ell)$ are $\ell$-dependent. We choose for the generator $\eta$

$$\eta(\ell) = \sum_i \left\{ \left[ (\mathcal{L} + \omega)A_i - \mu A_i^\dagger \right] b_i^\dagger + \left[ (\mathcal{L} - \omega)A_i^\dagger + \mu A_i \right] b_i \right\} \quad (7)$$

according to $\eta = [\mathcal{H}_S + \mathcal{H}_B, \mathcal{H}_{SB}]$. The general flow equation (2) leads to a flow equation for the coupling operator $A_i(\ell)$ by investigating the terms linear in phonon operators $[\eta(\ell), \mathcal{H}(\ell)]$

$$\frac{dA_i}{d\ell} = - \left\{ \left[ (\mathcal{L} + \omega)^2 - \mu^2 \right] A_i - 2\mu \mathcal{L} A_i^\dagger \right\}. \quad (8)$$

Due to the complicated structure of Eq. (8) we restrict ourselves to a subspace of operators, which are allowed to appear in $A_i(\ell)$. A systematic choice is to consider all terms arising in $A_i(0)$ and $\mathcal{L} A_i(0)$. The following table summarizes the resulting set of operators.

| coefficient | spin operator |
|-------------|---------------|
| $a(\ell)$   | $S_i S_{i+1} - S_i S_{i-1}$ |
| $b_0(\ell)$ | $iS_i S_{i+1} S_{i+2}$ |
| $b_1(\ell)$ | $iS_i S_{i+1} S_{i+2} + S_{i-1} S_i S_{i+1}$ |
| $b_2(\ell)$ | $iS_i S_{i+1} S_{i+3} + S_{i-3} S_{i-1} S_i$ |
| $b_3(\ell)$ | $iS_i S_{i+1} S_{i+2} S_{i+3} + S_{i-3} S_{i-1} S_i S_{i+1}$ |

In next order in $\mathcal{L}$ the operators arising in $\mathcal{L}^2 A_i(0)$ are included leading to 14 additional three spin operators of the type $(S_i \times S_j)(S_k \times S_l)$ and five additional long range two spin operators. Eq. (8) can now be divided in a set of differential equations for the spin-phonon coupling constants $a(\ell)$ and $b_n(\ell)$.

The truncation of the coupling operator $A_i$ in order $n$ (by constructing the operator space with all terms appearing in $A_i(0)$, $\mathcal{L} A_i(0)$, $\mathcal{L}^2 A_i(0)$, ..., $\mathcal{L}^n A_i(0)$) neglects effects of order $n + 1$ in $J$. We note here, that in this step no expansion in $g$ occurs. As the contribution to the flow of the neglected operators corresponding to higher order contributions in $J$ is small compared to the one of the leading order terms, we expect the flow equations to converge for $\ell \rightarrow \infty$. This actually is the case except for large values of $J/\omega$.

For the phonon frequencies we find

$$\frac{d\omega}{d\ell} = \langle \sum_i \left[ ((\mathcal{L} + \omega)A_i A_i^\dagger + [A_i, -\mathcal{L} + \omega] A_i^\dagger) \right] \rangle \quad (9a)$$

$$\frac{d\mu}{d\ell} = 2\langle \sum_i [\mathcal{L} A_i - \mu A_i A_i^\dagger] \rangle. \quad (9b)$$

Only nearest and next-nearest neighbour spin products are kept and their mean field value, denoted by the outer brackets $\langle \cdot \rangle$, is inserted.
The flow equations for $J_1(\ell)$ and $J_2(\ell)$ can be extracted from $[\eta, \mathcal{H}_{SB}]$

\[
\sum_i \left\{ \left[ (\mathcal{L} + \omega)A_i, A_i^\dagger \right] + \text{h.c.} \right\} \langle b^\dagger b \rangle \\
+ \sum_i \left\{ \left[ \mathcal{L}A_i - \mu A_i^\dagger, A_i \right] + \text{h.c.} \right\} \langle b^\dagger b^\dagger \rangle \\
- \sum_i \left\{ A_i^\dagger \left[ (\mathcal{L} + \omega)A_i - \mu A_i^\dagger \right] + \text{h.c.} \right\} .
\]

The quadratic boson terms are replaced by their expectation values. This is systematic in the sense of an expansion in $g$. This mean-field step neglected fluctuation effects of order $g^2$. As these terms only arise in $g^2$-terms, the total error is of order $g^2$ (cf. Ref. [6]). We note here, that these expectation values are $\ell$-dependent due to the $\ell$-dependence of $\omega$ and $\mu$. Finally, $\frac{d\eta}{dt} (\frac{d\mu}{dt})$ is equal to the (next) nearest neighbour part of (10), respectively.

$$\text{FIG. 1.: } \ell\text{-dependent flow of the the coupling constants, the phonon frequencies and the coefficients in the ansatz for the coupling operator } A \text{ in units of } \omega_0.$$  

$$\text{III. RESULTS}$$

Having collected all flow equations, the set of differential equations (9 in order $\mathcal{L}$ and 28 in order $\mathcal{L}_2$) have to be solved numerically. This is done via a standard fifth-order Runge-Kutta routine with adaptive step size control. The change of the $\ell$-dependent coupling constants for two succeeding Runge-Kutta steps is computed for all couplings. Convergence is assumed if the sum of the changes squared is less than $10^{-9}$ in units of $\omega_0$. Fig. 1 shows for $J/\omega_0 = 0.6$ and $g/\omega_0 = 0.3$ the flow of all 9 parameters. For intermediate values of $\ell$ the additional four spin coupling terms arise ($b_n(\ell) \neq 0$). As $\ell$ becomes larger, all spin-phonon coupling constants vanish, i.e. $\mathcal{H}_{SB} \rightarrow 0$. $J_1$ and $J_2$ reach their effective values in the limit $\ell \rightarrow \infty$ and thus give rise to a frustration $\alpha_{eff} = J_2^{eff}/J_1^{eff}$ in the decoupled spin model. This procedure is very intuitive in the sense that a flow diagram like

$$\text{FIG. 2.: Effective phonon frequencies } \omega_{eff} \text{ (thin lines in the upper part), } \mu_{eff} \text{ (lower part) and } \lambda_{ph} \text{ (thicker lines) for fixed values of the initial next-nearest neighbour coupling } J = J_1(\ell = 0), \text{ } \lambda_{ph} = \sqrt{\omega_{eff}^2 - \mu_{eff}^2} \text{ is the phonon frequency in the diagonalized version of the pure phonon part } \mathcal{H}_B.$$  

Fig. 1 shows, how the dressing of the spins with phonons induces a frustration $\alpha_{eff} > 0$.

As a by-product, we find an increased phonon frequency in the effective phonon part of the model. This phonon hardening can be interpreted qualitatively as a level repulsion between the high energy phonon system and the low energy spin system. Recently, it has been pointed out by Gros and Werner [18] that this feature is consistent with the RPA-approach by Cross and Fisher to the spin-Peierls transition. Fig. 2 shows for four values of $J$ the effective phonon frequencies in dependence of $g$. As an appropriate measure of the phonon hardening, the frequency $\lambda_{ph} = \sqrt{\omega_{eff}^2 - \mu_{eff}^2}$ of the diagonalized version $\mathcal{H}_B \rightarrow \sum_i \lambda_{ph} \beta_i^\dagger \beta_i + \lambda_{ph,0}$ is depicted.

The phase diagram of the spin-Peierls anti-ferromagnetic chain of spins interacting with phonons has been investigated by Bursill et al. via DMRG [9], by Uhrig via flow equations in leading order in $g/\omega$ and $J/\omega$ [19], by Weiße et al. via fourth order perturbation theory and Lang-Firsov transformation [20] and by Sun et al. via mean field and renormalization group methods [21]. In Fig. 3 results of various flow equation approaches are shown. In Fig. 4, we compare our results to those of the other approaches.

Our calculation is based on the idea that the transition into the ordered phase does not occur due to the softening of a phonon but due to the tendency of the effective spin model towards dimerization. Phonon-induced frustration above its critical value $\alpha_{eff} > \alpha_c$ drives the dimerization. The phase transition line is therefore determined by solving

$$\alpha_c - \left( \lim_{\ell \rightarrow \infty} \alpha \right)_{g,J} = 0$$

for fixed values of $J$ with respect to $g$. In this way we
find the critical spin-phonon coupling \( g_c \) in dependence of the nearest neighbor spin coupling \( J \). For values of \( J/\omega \) up to 0.35 the extended flow equation approach improves the results from Ref. [6]. For intermediate values of \( J/\omega \) the curve crosses the DMRG result and predicts critical couplings, which must be considered as too low. It is interesting that the result of Ref. [6] gives a good description of \( g_c \) up to \( J/\omega \approx 10 \) although it is systematic only to order \( g^2/\omega^2 \) and \( g^2J/\omega^3 \). We presume that the two leading orders comprise already the main competition between dimerization and delocalization. Further orders start to build in resonance effects. But they do not succeed for all \( J/\omega \) because the effective interactions are restricted to small distances only in our ansatz. It is not uncommon (cf. mean field treatments) that the leading orders yield physically reasonable though not accurate results whereas systematic improvements are difficult to implement (see Ref. [22] for an expansion in the inverse coordination number as example).

The inclusion of the next order in the systematic expansion by Weiße et al. leads to slight improvements for \( J/\omega < 0.15 \) which is an estimate of the convergence radius of the series expansion. But the higher order terms produce too large critical couplings even for intermediate values of \( J/\omega \) [20]. Furthermore, Weiße et al. used the Lang-Firsov transformation to combine adiabatic and antiadiabatic effects in their theory. This leads actually to an additional increase of the critical couplings for intermediate \( J/\omega \) (cf. Fig. 6 in Ref. [15]). We conclude that the extended flow equation approach used here has important advantages over the systematic series expansion. This is due to its renormalizing property, i.e. the feedback of the \( \ell \)-dependence of all couplings. In this way the region of validity is increased up to \( J/\omega \approx 0.35 \).

### IV. Modifications

To enlarge the region of validity of the flow equation approach to larger \( J \)s, we introduce some modifications. In a first attempt the restriction to a given operator subspace can be dropped for intermediate terms arising in (8-10) via \( \mathcal{A}_\ell \). This circumvents the downturn of the phase transition line but leads to too large critical couplings \( g_c(J) \). As these modifications changed the solutions of the differential equations drastically the influence of longer range interactions present in these intermediate terms can be judged as important. To include them in

![FIG. 3: Zero temperature phase diagram of the spin-Peierls antiferromagnetic chain of spins interacting with phonons. For small values of the spin-phonon coupling \( g/\omega \), the system is gapped. For large \( g/\omega \), the system is dimerized and has an energy gap. The curves denoted with \( \alpha^{\text{sw}} \) and \( d^{\text{sw}} \) are the results of two modified approaches and will be discussed in Chapter IV.](image)

![FIG. 4: Phase diagram like Fig. 3. Various previous results are compared with the phase transition lines obtained via flow equations or DMRG. For values of \( J/\omega < 1 \) Sun et al. use \( g_c/\omega = \sqrt{J/(2\omega)} \) [21, 23]. This is smaller by about a factor \( 1/\sqrt{2} \) than the first order result obtained by Kuboki and Fukuyama [24], who find \( g_c/\omega = \sqrt{\alpha_c/(1/2 - \alpha_c)} \cdot J/\omega \approx \sqrt{J/\omega} \). As can be seen from Figure 4, the results of Sun et al. do not compare so well with those of the other approaches. For \( J/\omega > 2 \) they find critical couplings \( g_c/\omega \approx 0.6 \), which are about twice as large as the \( g_c \)-values computed by DMRG [9]. For increasing \( J/\omega \), Sun et al. predict decreasing \( g_c \) above \( J/\omega \approx 5 \) (not shown) in contrast to the DMRG data.

While for not too large values of \( J/\omega \) the extension of the flow equation approach to higher orders in \( g/\omega \) provides a fast method to retrieve data as precise as DMRG calculations, the large \( J/\omega \) regime cannot be described so easily. At \( J/\omega \approx 0.77 \) the effective Hamiltonian is no longer hermitian and the description breaks down. The next systematic extension is to enlarge the operator subspace for \( \mathcal{A}_\ell \) to order \( \mathcal{L}^2 \). The result once again improves the calculations in order \( \mathcal{L} \) for small \( J/\omega \), but cannot circumvent the “downturn” at \( J/\omega \approx 0.4 \). We will argue below that the inclusion of longer range interactions is necessary for \( J/\omega > 0.35 \).
a systematic way two additional couplings $J_3$ and $J_4$ are introduced. They correspond to spin interactions $S_iS_{i+3}$ and $S_iS_{i+4}$. The flow equations for $J_2(\ell)$ and $J_4(\ell)$ can be extracted from (10). As the critical coupling $\alpha_c$ is only known for the $J_1$-$J_3$-model we combine these four couplings to two effective couplings $J_{1w}^{\text{sw}}(\ell)$ and $J_{2w}^{\text{sw}}(\ell)$ and thus $\alpha^{\text{sw}}(\ell) = \frac{J_{1w}^{\text{sw}}}{J_{1w}^{\text{sw}}} / \frac{J_{2w}^{\text{sw}}}{J_{2w}^{\text{sw}}}$. This is done by using linear spin wave theory [25]. The effective couplings $J_{1w}^{\text{sw}}$ and $J_{2w}^{\text{sw}}$ are chosen such that the spin wave dispersion with $J_{1w}^{\text{sw}}$ and $J_{2w}^{\text{sw}}$ equals the one for $J_1$, $J_2$, $J_3$ and $J_4$. Thus we obtain

$$J_{1w}^{\text{sw}} = \sqrt{(J_1 + 9J_3)(J_1 + J_3)}$$

$$J_{2w}^{\text{sw}} = \sqrt{\frac{J_1 + J_3}{J_1 + 9J_3}(J_2 + 4J_4)}$$

$$\alpha^{\text{sw}} = \frac{J_{2w}^{\text{sw}}}{J_{1w}^{\text{sw}}} = \frac{J_2 + 4J_4}{J_1 + 9J_3}$$

(12a)

(12b)

(12c)

The curve of Fig. 3 denoted with $\alpha^{\text{sw}}$ is the solution of $\alpha_c - \alpha^{\text{sw}} = 0$. The downturn does not occur any more, but the critical couplings are too large. As $\frac{d\alpha^{\text{sw}}}{d\ell}$ and $\frac{d^2\alpha^{\text{sw}}}{d\ell^2}$ are solved separately from all other coupling constants, i.e. $J_3$ and $J_4$ do not couple to the other differential equations, another method denoted with $\alpha^{\text{sw}}$ is introduced. Differentiating (12a) and (12b) one finds $\frac{dJ_{1w}^{\text{sw}}}{d\ell}$ and $\frac{dJ_{2w}^{\text{sw}}}{d\ell}$. These two derivatives do depend on all $J_n$ and $\frac{dJ_n}{d\ell}$ ($n = 1, \ldots, 4$). They are calculated in each Runge-Kutta step. This provides a coupling of $J_3$ and $J_4$ to the other flow equations. The results from this procedure show again the downturn at $J/\omega \approx 0.4$ and produce worse data for small $J/\omega$ than the unmodified approach.

The inclusion of long range interaction terms modifies the results drastically. So they are important and have to be treated correctly. It seems that one has to extend the flow equation approach to very high orders in the Liouville operator $\mathcal{L}$, i.e. the subspace for the coupling operator $\mathcal{A}_i(\ell)$ should be fairly large, if one wants accurate data for large values of $J/\omega$. For $J/\omega < 0.35$, however, the method presented works very accurately.

Due to the complicated spin commutators and products in the flow equations an extension to higher orders in $\mathcal{L}$ is cumbersome. A further hint of how this could be achieved more easily shall be given. Recently non-standard choices of the generator $\eta$ have been used successfully [26, 27]. The main point is to introduce a quantum number $Q$ and define the generator via $\eta(\ell) = [Q, \mathcal{H}(\ell)]$. Thus $[\mathcal{H}_{\text{eff}}, Q] = 0$, i.e. $Q$ is conserved with respect to $\mathcal{H}_{\text{eff}}$. For our problem we introduce the phonon number $Q = \sum_i b_i^\dagger b_i$. With this choice the generator reads $\eta = \sum_i [A_i b_i^\dagger - A_i^\dagger b_i]$ and does not contain the Liouville operator. The flow equations (for $T = 0$) are pretty simple

$$\frac{dA_i}{d\ell} = -(\mathcal{L} + \omega)A_i$$

$$\frac{d\omega}{d\ell} = 2([A_i, A_i^\dagger])$$

$$[\eta, \mathcal{H}_{\text{SB}}] = -2 \sum_i A_i^\dagger A_i .$$

(13a)

(13b)

(13c)

We investigated these flow equations in order $\mathcal{L}$ and $\mathcal{L}^2$. The results are similar to those of the standard choice of $\eta$. Although the standard choice (3) leads to slightly better results for small couplings $J/\omega$, the alternative generator could be used to investigate very large subspaces for $\mathcal{A}_i(\ell)$, as only $\mathcal{L}$ enters linearly in (13a) and it is absent in (13b,13c).

V. SUMMARY

We used the flow equation method to rotate the spin-phonon coupling of a spin-Peierls Hamiltonian away. In this way we derived effective spin and phonon models. The spin-phonon coupling induces longer range interactions, i.e. produces a non-vanishing frustration, and renormalizes the original couplings. The effective phonon frequency is enlarged. This corresponds to the phonon hardening observed for CuGeO$_3$. The phase diagram describing the transition from a gapped to an ungapped state is compared with DMRG results. For large values of $J/\omega$ the results deviate. In this regime very long range interactions appear to be relevant and the transformation of the spin-Peierls chain onto a rather local effective spin model must be considered as not sufficient. The flow equation and the DMRG results coincide for $J/\omega < 0.35$.

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