Spin-wave theory for dimerized ferromagnetic chains

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Abstract. We describe a Peierls dimerization which occurs in ferromagnetic spin chains at finite temperature, within the modified spin-wave theory. Usual spin-wave theory is modified by introducing a Lagrange multiplier which enforces a nonmagnetic state at finite temperature. It is shown that this method gives results in excellent agreement with the density–matrix renormalization group applied to transfer matrices for dimerized ferromagnetic chains. We study bond correlation functions ⟨Sᵢ · Sᵢ₊₁⟩ and explore the characteristic features of dimerization in the specific heat.

1. Introduction
It is a well established fact that a coupling between electronic and lattice degrees of freedom can drive structural instabilities of electronic systems. This effect is induced by a gain in electronic energy surpassing the cost in elastic energy due to the lattice distortion. For instance, in the Peierls instability, a static lattice distortion turns a one-dimensional (1D) free electron system into a band insulator [1]. A similar effect has been observed for antiferromagnetic (AFM) spin chains coupled to phonons where a gain in magnetic energy drives the so-called spin-Peierls transition [2]. A further example for a Peierls instability, where a ferromagnetic (FM) spin-chain shows a periodic modulation (dimerization) of the magnetic exchange in a certain finite temperature region was observed in YVO₃ [3] and has recently been discussed theoretically [4, 5]. This effect is induced by a coupling of the spin and orbital degrees of freedom [6].

In this paper we highlight the differences of the spin-Peierls transition in AFM and FM spin chains and discuss the dimerized FM spin chain within the framework of modified spin-wave theory (MSWT). We show that this method yields results in excellent agreement with numerical data [5]. In particular, we consider the specific heat and bond correlation functions. In addition we give an analytical expression for the free energy at low temperatures and small dimerization allowing for a quantitative understanding of the occurrence of dimerization in FM spin chains.

2. Spin-Peierls effect in spin chains
First, we investigate under which circumstances a Peierls dimerization may occur in FM spin chains. It will be also instructive to discuss briefly the Peierls dimerization in AFM spin chains to highlight the differences between the FM and AFM case.

Our starting point is a coupling of the spin chain to lattice degrees of freedom. If the Peierls gap exceeds the phonon frequency it is permissible to neglect the phonon fluctuations. Within
where we have defined \( \delta \equiv 2gu/(Ja_0) \) and \( K \equiv \tilde{K}J^2a_0^2/(4g^2) \). Here \( J \) is the exchange constant, \( S_j \) a spin \( S \) operator at site \( j \), \( N \) the number of sites, and \( K \) the effective elastic constant with \( E_{el} = N\tilde{K}u/2 \). The dimensionless parameter \( \delta \) is given by the exchange constant \( J \), the spin-phonon coupling constant \( g \), the atomic displacement \( u \), and the lattice constant \( a_0 \). We note that in spite of the fact that the model (1) is 1D, the static, mean-field treatment of the three-dimensional phonons allows for a finite temperature phase transition if \( \delta(T) \) is treated as a thermodynamical degree of freedom.

For the 1D Heisenberg antiferromagnet it was shown that \( E_{mag} \sim -\delta^{4/3} \) \[7\]. Hence the cost in elastic energy due to a distortion of the lattice is outweighed by the contribution stemming from the magnetic part of the Hamiltonian. This leads to a spin-Peierls transition for every value of \( K \) at sufficiently low temperature. The phase diagram obtained within the density-matrix renormalization group applied to transfer matrices (TMRG) \[8\] is shown in figure (1a) for the dimerized AFM \( S = 1/2 \) Heisenberg chain (1). The phase transition is of second order. The inset shows the parameter \( \delta \) as a function of temperature.

In figure (1b) the phase diagram for the dimerized FM chain obtained by TMRG is shown. We observe that a dimerized phase exists only at \( T > 0 \) and only if \( K/|J| < K_c/|J| \approx 0.118 \). We also report a tricritical point (TCP) at \((T_{TCP}/|J|, K_{TCP}/|J|) \approx (0.696, 0.116)\). For \( T < T_{TCP} \) and \( T > T_{TCP} \) the transition will be first and second order, respectively. This is shown in the inset of figure (1b) where we can see that at the upper phase boundary \( \delta(T) \) evolves continuously.

3. Modified spin-wave theory for dimerized chains

For the case of a FM chain, we apply a Holstein-Primakoff transformation onto the magnetic part of Hamiltonian (1). Since the unit cell is doubled for the dimerized chain we have to distinguish between magnons on two sublattices. Hence we write

\[
S_j^+ = \sqrt{2S - a_{j\alpha}^\dagger a_{j\alpha}} \quad \text{and} \quad S_j^- = a_{j\alpha}^\dagger \sqrt{2S - a_{j\alpha}^\dagger a_{j\alpha}} \quad \text{for the dimerized phase.}
\]

\[
S_{j,\alpha}^z = S - a_{j,\alpha}^\dagger a_{j,\alpha},
\]

(2)
where $a_{ja}$ and $a_{ja}^\dagger$ are bosonic annihilation and creation operators at site $j$. The index $\alpha \in \{e, o\}$ refers to the sublattice for $j$ being an even ($e$) or an odd ($o$) index, respectively. Retaining only the lowest order terms we obtain a bilinear Hamiltonian which can be diagonalized by means of a Bogoliubov transformation. The diagonalized Hamiltonian reads

$$H_{\text{mag}} = H_0 + \sum_k (\omega_k^- a_k^\dagger a_k + \omega_k^+ \beta_k^\dagger \beta_k),$$

with $H_0 = -|J| S^2 N$ and the magnon branches $\omega_k^\pm = 2|J| S (1 \pm \sqrt{\cos^2 k + \delta^2 \sin^2 k})$ which are shown in figure 2(a).

The idea of Takahashi’s MSWT [9] is to retain Hamiltonian (3) while enforcing the Mermin-Wagner theorem. This is achieved by minimizing the free energy subject to the constraint that the magnetization at finite temperature vanishes. To this end a Lagrange multiplier is introduced serving as a chemical potential. Applying MSWT for the dimerized FM chain we obtain the constraint

$$S = \frac{1}{N} \sum_k \{n_B(\omega_k^-) + n_B(\omega_k^+)\},$$

with $n_B(\omega_k^\pm) = \{\exp[(\omega_k^\pm - \mu)/T] - 1\}^{-1}$ being the Bose factors. The free energy per site in this approximation reads

$$f = -|J| S + \mu S - \frac{T}{N} \sum_k \{\ln \left[1 + n_B(\omega_k^-)\right] + \ln \left[1 + n_B(\omega_k^+)\right]\}.$$

For the uniform case ($\delta = 0$) it reduces to the free energy obtained by Takahashi for the 1D Heisenberg ferromagnet [9].

The free energy can be obtained analytically within the MSWT framework in the limit $t_\delta \equiv T/\{|J| S (1 - \delta^2)\} \ll 1$. To this end we expand equation (4) [10] to obtain

$$v = t_\delta \left(1 + \alpha \sqrt{t_\delta} + \frac{3}{4} \alpha^2 t_\delta + \ldots\right),$$

with $v \equiv -4 \mu S^2 / T$, and $\alpha \equiv \zeta(\frac{1}{2}) / S \sqrt{\pi}$. Inserting this result into equation (5) we obtain $f = -|J| S - T \{\zeta(\frac{3}{2}) t_\delta^{3/2} / (2 \sqrt{\pi}) + \mathcal{O}(t_\delta)\}$. Hence the gain in magnetic energy is proportional $\delta^2$ as is the elastic energy, explaining the existence of a critical value $K_c / |J|$.

Due to the alternating interaction between the spins, nearest-neighbor correlation functions (NNCF) will also exhibit alternation in strength. Hence $\Delta_{SS} \equiv \langle S_{2j} \cdot S_{2j+1} \rangle - \langle S_{2j} \cdot S_{2j-1} \rangle$ serves as an order parameter for the dimerized chain. In calculating the corresponding NNCF within MSWT it is essential to also retain quartic bosonic terms which leads to

$$\langle S_{2j} \cdot S_{2j+1} \rangle = \left(\frac{1}{N} \sum_k \left[n_B(\omega_k^-) - n_B(\omega_k^+)\right] f_k^\pm(\delta)\right)^2,$$

with $f_k^\pm(\delta) = (\cos^2 k \pm \delta \sin^2 k) / (\sqrt{\cos^2 k + \delta^2 \sin^2 k})$. In figure 2(b) results from MSWT for $\Delta_{SS}$ as a function of $\delta$ at various temperatures are compared to those obtained within TMRG. The agreement is good up to $T / |J| \sim 1$ and even the right limit is captured by MSWT for the fully dimerized case. However, corrections $\delta = 1 - \epsilon$ are predicted to be of order $\epsilon^2$ for $\epsilon \ll 1$ whereas perturbation theory exhibits corrections of order $\epsilon$.

With equation (7) it is easy to determine the internal energy per site reading

$$u = \frac{1}{2} \left\{ (1 - \delta) \langle S_{2j-1} \cdot S_{2j} \rangle + (1 + \delta) \langle S_{2j} \cdot S_{2j+1} \rangle \right\}.$$
Using this result the specific heat per site reads
\[ c = c^+ + c^- \]
\[ c^\pm = \frac{(1 \pm \delta)}{T^2N^2} \sum_{k, k', \sigma \in \{\pm\}} (-\sigma)n_B(\omega_{k'}^\sigma)[1 + n_B(\omega_{k'}^\sigma)] \left( \omega_{k'}^\sigma - \mu + T \frac{\partial \mu}{\partial T} \right) f_k^\pm \{ n_B(\omega_k^-) - n_B(\omega_k^+) \} f_k^\pm \]  

In figure 2(c) we show the specific heat per site as a function of temperature for various dimerizations. For \( \delta = 0 \) we find one broad hump which still is retained if \( \delta \ll 1 \). However, at a higher dimerization we observe that the two magnon branches give distinct contributions leading to a sharp low temperature peak and a hump at higher temperatures stemming from well separated magnon excitations, see figure 2(a). The excitations of the lower magnon band \( \omega_k^- \) may occur at low \( T \) whereas those of the higher band \( \omega_k^+ \) contribute only when \( T \) is high.

4. Conclusions
We have discussed the differences in the occurrence of a spin-Peierls transition in AFM and FM spin chains. For the FM chain we have applied MSWT and found that the magnetic energy gain \( \sim -T^{3/2} \delta^2 \) directly competes with the cost in elastic energy. The dimerization order parameter obtained from MSWT is found to be in excellent agreement with TMRG data. Finally, we have shown that dimerization leads to a qualitatively different behaviour of the specific heat.

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