Molecular-field approach to the spin-Peierls transition in CuGeO₃

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We present a theory for the spin-Peierls transition in CuGeO₃. We map the elementary excitations of the dimerized chain (solitons) on an effective Ising model. Inter-chain coupling (or phonons) then introduces a linear binding potential between a pair of soliton and anti-soliton, leading to a finite transition temperature. We evaluate, as a function of temperature, the order parameter, the singlet-triplet gap, the specific heat, and the susceptibility and compare with experimental data on CuGeO₃. We find that CuGeO₃ is close to a first-order phase transition. We point out, that the famous scaling law $\delta^{2/3}$ of the triplet gap is a simple consequence of the linear binding potential between pairs of solitons and anti-solitons in dimerized spin chains.

I. INTRODUCTION

With the discovery of the first inorganic spin-Peierls compound CuGeO₃ it has become possible to investigate the physics of the spin-Peierls transition in quasi one-dimensional spin chains with high precision. Of particular interest has been the study of the magnetic excitation spectrum by neutron scattering and Raman scattering experiments. It has been observed that the spin-Peierls gap, i.e. the gap to triplet excitations out of the singlet ground-state, has a temperature dependence which is difficult to explain with existing theories of the spin-Peierls transition.

Existing theories of the spin-Peierls transition of spin-1/2 Heisenberg chains are based on the mapping of the spin chain to an interacting gas of spin-less fermions via the Jordan-Wigner transformation. The chains are coupled to a three-dimensional phonon mode and the transition occurs when the respective phonon frequency becomes soft. In the spin-Peierls state the unit-cell doubles due to the alternating displacements of the magnetic ions. The effective Hamiltonian for the magnetic excitations along the chains in the dimerized state is then

$$H = J \sum_i \left[ (1+\delta(-1)^i) \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]. \quad (1)$$

The nearest neighbor (NN) exchange has alternating strength $J(1 \pm \delta)$ due to the doubling of the unit cell below the spin-Peierls transition temperature $T_{SP}$. Also included is a frustrating next-nearest-neighbor (NNN) term $\sim J\alpha$. The ground-state phase diagram of CuGeO₃ has been mapped out by a density matrix renormalization group study. There is a gap everywhere in the phase-diagram except on the line $\delta = 0$ and $\alpha < \alpha_c$, with $\alpha_c \approx 0.2411$. A vividly debated question of key interest is therefore the actual magnitude of the strength of the frustration $\alpha$. For CuGeO₃ the parameters have been estimated as $J \approx 150\text{–}160$K and $\alpha \approx 0.24\text{–}0.3$.\cite{Cox95}

A consequence of existing theories of the spin-Peierls transition is the occurrence of a soft phonon mode above $T_{SP}$, which has not yet been observed for CuGeO₃.\cite{Kodama93}

It is therefore of interest to pursue the possibility of a purely electronically driven spin-Peierls transition, as it could occur for $\alpha > \alpha_c$. In such a scenario the phonons would just follow the pre-formed electronic dimerization, i.e. the formation of NN singlet pairs. Here we propose a simple molecular-field type theory for the spin-Peierls transition by mapping the low-energy solitonic excitations of dimerized spin chains on an effective Ising model. We emphasize that this procedure is valid both for the phonon-driven and for the electronically-driven spin-Peierls transition. We present results of the mean-field theory in comparison with experiments on CuGeO₃.

We find that a straightforward determination of the frustration parameter $\alpha$ is not conclusive and that CuGeO₃ is close to a first-order phase transition. We also note that the famous $\delta^{2/3}$ scaling of the triplet gap is a simple consequence of the linear binding potential between solitons and anti-solitons in dimerized spin chains.

II. MAPPING ON AN EFFECTIVE ISING MODEL

A strictly one-dimensional system shows no long-range order at finite temperatures due to the solitonic excitations. The appropriate solitons in a spin-Peierls state are domain-walls in between two different dimer coverings, see Fig.\cite{Werner97}. In this picture a dimer consists of a NN pair of spins in singlet state. A single soliton in an otherwise (dimer-) ordered chain is in reality a complicated object. It is spatially extended and has a spin degree of freedom together with a dispersion, which in the Majumdar-Gosh model ($\alpha = 1/2$) has the form $J(5/4 - \cos 2k)$. It has been shown\cite{Kodama93} that the solitons yield an accurate description of the magnetic susceptibility and hence of the Hilbert space.

The dispersion of the solitons might be approximated, in general, by

$$E(k) = \sqrt{(E_s)^2 + (cJ \sin k)^2}, \quad (2)$$

where $E_s$ is the gap to solitonic excitations, $J$ the exchange integral, $c$ a constant of order of unity, and
**III. EXCITATION ENERGIES**

We have two relevant excitation energies, the gap to single soliton excitations, given by \( E_s \) in (3), and the gap to triplet excitations, \( \Delta_N \), as measured in a neutron scattering experiment. Let us now discuss the relation of \( \Delta_N \) to \( E_s \).

\[ k \text{ is the wavenumber in units of inverse lattice spacings. Only the low-energy solitons are effective in destroying the long-range dimer order, and we approximate here (3) by a constant } E(k) \equiv E_s. \text{ We will furthermore not discuss the consequence of the spatial extent of the solitons and we will include their spin-degree of freedom only when determining the susceptibility. We take one of the two possible dimer configurations of the linear chain as the reference state and label every “good” dimer by +1 and every bond between two “wrong” dimers by −1; A bond between a soliton and a wrong dimer is also labeled −1 as shown in Fig. I. Every possible soliton configuration is therefore mapped to a Ising-spin configuration living on every second bond. A similar mapping has been used recently by Mostovoy and Khomskii.} \]

\[ \text{FIG. 1. Phenomenological picture of copper chains in CuGeO$_3$. a): A soliton and an anti-soliton in a dimerized chain with the corresponding values of the dimer operators } \sigma_{i,l}. \text{ There is one dimer operator for every pair of sites. b) and c): Illustration of two different dimer configurations which lead to an inter-chain coupling contribution to the energy of } \pm 0.5\Delta_g. \text{ The origin of the coupling may be attributed to the inter-chain exchange as well as to phononic effects.} \]

We now consider a two-dimensional array of chains and define by \( \sigma_{i,l} = \pm 1 \) the Ising variable on the \( l \text{th} \) chain, where the site index \( i \) runs over every second bond of a chain of length \( L \). Including a coupling \( \Delta_g \) between dimers on NN chains we have

\[ H_{2D} = E_s \sum_{i,l} \frac{1}{2} (1 - \sigma_{i,l} \sigma_{i+1,l}) - \frac{\Delta_g}{2} \sum_{i,l} \sigma_{i,l} \sigma_{i,l+1} \]  

\[ \text{(3)} \]

as the effective Ising Hamiltonian. The inter-chain coupling \( \Delta_g \) might be induced by the inter-chain exchange coupling, \( J_{ll} \approx 0.1J \). In this case \( \Delta_g \sim (J_{ll})^2/J \). An indirect coupling of the chains via phonons is also conceivable. It has been shown recently, that a molecular-field decoupling of inter-chain interactions in quasi one-dimensional systems is a good approximation in the strongly anisotropic limit. We may therefore decouple the chains via

\[ \sigma_{i,l} \sigma_{i+1,l} \rightarrow \sigma_{i,l} \langle \sigma_{i+1,l} \rangle + \sigma_{i+1,l} \langle \sigma_{i,l} \rangle - \langle \sigma_{i,l} \rangle \langle \sigma_{i+1,l} \rangle, \]

\[ \text{(4)} \]

where the \( \langle \sigma_{i,l} \rangle \) denotes the thermodynamic expectation value. Translational invariance perpendicular to the chains yields \( \langle \sigma_{i+1,l} \rangle = \langle \sigma_{i,l} \rangle = \langle \sigma \rangle \) and the Hamiltonian for a single chain (the number of Ising variables is \( L/2 \)) becomes in this mean-field approximation

\[ H = -\frac{1}{2} E_s \sum_{i=1}^{L/2} \sigma_i \sigma_{i+1} - B \sum_{i=1}^{L/2} \sigma_i + \frac{L}{4} E_s + \frac{L}{4} \Delta_g \langle \sigma \rangle^2, \]

\[ \text{(5)} \]

where we have set \( B = \Delta_g \langle \sigma \rangle \). This is just the Ising Hamiltonian for a ferromagnetic spin chain in an external magnetic field \( B \). Alternatively we can interpret (3) as an effective model for domain walls in a spin-Peierls state with a linear binding potential \( V(x) = B \cdot (x + 1) \) (with \( x \geq 1 \) being the distance in sites, not bonds) between a soliton and an anti-soliton.

So far we have neglected the spin-phonon coupling \( \lambda_{sp} \). A finite value for the spin-singlet order parameter \( \langle \sigma \rangle \) leads through \( \lambda_{sp} \) to a finite lattice dimerization and consequently to a modulation of the exchange constant, \( J(1 + \delta) \), in (I), with \( \delta \sim \lambda_{sp} \langle \sigma \rangle \). The spin-phonon coupling therefore adds a term \( \sim \lambda_{sp} \langle \sigma \rangle \) to the confining potential \( B \). On a mean-field level this corresponds to a rescaling of the coupling constant

\[ \Delta_g \rightarrow \Delta_g + c_1 \lambda_{sp}, \quad B \rightarrow B + c_2 \delta, \]

\[ \text{(6)} \]

with appropriate constants \( c_1 \) and \( c_2 \).

The partition function \( Z \) can be obtained from (2) by the transfer matrix method. The free energy \( F = -k_B T \ln Z \) is given in the thermodynamic limit \( (L \to \infty) \) by

\[ \frac{F}{L/2} = -k_B T \ln \lambda_0 + \frac{1}{2} \Delta_g \langle \sigma \rangle^2 \]

\[ \text{(7)} \]

where

\[ \lambda_0 = \cosh(\beta \Delta_g \langle \sigma \rangle) + \sqrt{\sinh^2(\beta \Delta_g \langle \sigma \rangle) + e^{-2\beta E_s}}, \]

\[ \text{(8)} \]

with \( \beta = 1/(k_B T) \) being the inverse temperature. From the free energy all physical quantities can be derived.
A triplet excitation can dissolve into a soliton/anti-soliton pair. The linear binding energy $V(x) = B(x+1)$ in between a soliton and an anti-soliton in [3] leads to a confinement of soliton/anti-soliton pairs. In [3] we have neglected the kinetic energy of the single solitons [4], which is of order $J$. The energy levels of a particle in a linear confining potential are well known [5]. The lowest eigenstate has, in the limit $B \ll J$, the energy

$$\Delta_N = 2E_s + c'J \left(\frac{B}{J}\right)^{2/3},$$  

with $c' \approx 2.33$. Eq. (9) gives then the gap to triplet excitations as a function of soliton energy $E_s$ and the strength of the confining potential $B$. The mean extension of a soliton/anti-soliton pair scales like $(B/J)^{-1/3}$. For $\alpha < \alpha_c$ we have $B \rightarrow c_2\delta$ and Eq. (8) takes then the form

$$\Delta_N^{(0)} \approx 2E_s + 2.33v_s \left(\frac{c_2\delta}{v_s}\right)^{2/3},$$

where $v_s \approx (\pi/2)(1 - 1.12\alpha)L$ is the $\alpha$-dependent spin-wave velocity [4]. It is known [3], that the gap scales for $\alpha < \alpha_c$ like $\sim \delta^{2/3}$ implying that $E_s\delta^{-2/3} \rightarrow 0$ for $\delta \rightarrow 0$. Comparison with numerical results leads to $c_2 \approx 0.85$. The functional form of the dependence of the triplet excitation energy $E_s$ on $\delta$, or alternatively on the dimerization order parameter $\langle \sigma \rangle$ is not known at present. It might be extracted for $\alpha < \alpha_c$, in principle, from a sub-leading scaling analysis of the excitation energy

$$\Delta_N = \tilde{c}J \delta^{2/3} + 2E_s(\delta),$$

but this has not yet been done. We have therefore decided to assume the functional form

$$E_s(\langle \sigma \rangle) = E_\infty + (E_0 - E_\infty)\langle \sigma \rangle^2,$$

where $E_0$ is the zero-temperature value of $E_s$ and where $E_\infty$ is the soliton energy in the disordered phase, i.e. for $T > T_{SP}$. Eq. (9) is, in the spirit of a Landau functional [6], the simplest form consistent with the symmetry of $\langle \sigma \rangle$.

### IV. LANDAU EXPANSION

We may expand the free energy [6] in powers of $\langle \sigma \rangle$,

$$F = F_0 + a(T)(\langle \sigma \rangle)^2 + b(T)(\langle \sigma \rangle)^4 + O(\langle \sigma \rangle^6).$$

Depending on the parameters we may have either a second-order phase transition with $b(T) > 0$ or a first-order phase transition with $b(T) < 0$. In the first case the transition temperature $T_{SP}$ is given by $a(T_{SP}) = 0$ as

$$k_BT_{SP} = \frac{\Delta_g^2(1 + e^{-\beta E_\infty})}{2(E_0 - E_\infty)e^{-2\beta E_\infty} + \Delta_g(1 + e^{-\beta E_\infty})e^{-\beta E_\infty}},$$

with $\beta \rightarrow 1/(k_BT_{SP})$. This transcendental equation takes a simple form in some limiting cases:

$$E_\infty = 0 : \quad T_{SP} = \frac{\Delta_g^2}{\Delta_g + E_0}$$

$$E_\infty = E_0 : \quad T_{SP} = \frac{E_0}{\Delta_g e^{-\beta E_0/(k_BT_{SP})}}$$

$$\Delta_g \rightarrow \infty : \quad T_{SP} \rightarrow \Delta_g - E_0 + 2E_\infty$$

For illustration we present in Fig. 2 (a) $T_{SP}$ as a function of the inter-chain coupling constant $\Delta_g$ for $E_0 = 0.2\text{meV}$.

![Critical temperature vs. interchain coupling difference](image)

### FIG. 2. (a): Illustration of the spin-Peierls transition temperature $T_{SP}$ for $E_0 = 0.2\text{meV}$ as a function of $\Delta_g$. (b): Phase diagram as a function of $E_\infty$ and $E_0$ for fixed $T_{SP} = 14.15K$. Only the region $E_0 > E_\infty$ is allowed (above the solid line). Above the dashed line the phase transition is of first-order, below it is of second-order. The crosses indicate the parameter values considered for comparison with CuGeO$_3$.  

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For \( b(T_{SP}) < 0 \) we obtain a first-order phase transition. This is the case for values of \( E_0 \) larger than a certain critical value of the soliton energy \( E_c \), which is determined from \( b(T_{SP}) = 0 \) as

\[
E_c = E_∞ + \frac{Δ^2}{T_{SP}} \left( 1 + e^{E_∞/T_{SP}} \right)^2 \left( \sqrt{\frac{1 + 3e^{E_∞/T_{SP}} + 3e^{2E_∞/T_{SP}}}{6(1 + e^{E_∞/T_{SP}})^2}} - \frac{1}{2} \right). \tag{16}
\]

For a fixed transition temperature \( T_{SP} = 14.15K \) and using Eq. (14), \( E_c \) and the corresponding inter-chain coupling energy \( Δ_g \) can be calculated as a function of \( E_∞ \). The resulting phase diagram is given in Fig. 2(b). The numerical results presented throughout this paper are obtained within the second-order regime, indicated by the crosses in Fig. 2(b).

V. SELF-CONSISTENCY EQUATION

The effective Hamiltonian Eq. (3) contains three free parameters, namely \( E_∞, E_0 \) and \( Δ_g \). We examine two scenarios. The first is the case of \( α_c > α \) with \( E_∞ = 0 \). The second is the case of \( α_c < α \approx 0.35 \) with \( E_∞ = 0.15\text{meV} \) corresponding to a gap in the disordered phase of \( 2E_∞ = 0.3\text{meV} \). For each case we consider a range of \( E_0 \) (see Fig. 2(b)) within the second-order regime, \( E_∞ ≤ E_0 ≤ E_c \).

\[
E_∞ = 0 \text{meV}; \quad E_0 = 0, 0.1, 0.2, 0.277 \text{meV} \tag{17}
\]

\[
2E_∞ = 0.3 \text{meV}; \quad E_0 = 0.15, 0.3, 0.4, 0.474 \text{meV} \tag{18}
\]

The largest value of \( E_0 \) for each \( E_∞ \) corresponds to \( E_c(E_∞) \), compare Fig. 2(b). The experimental transition temperature \( T_{SP} = 14.15K \) of CuGeO₃ then determines the coupling constant \( Δ_g \).

The order parameter \( \langle σ \rangle \) is determined self-consistently as a function of temperature by setting the derivative of the free energy with respect to \( \langle σ \rangle \) to zero,

\[
\langle σ \rangle = \frac{\sinh(βΔ_g\langle σ \rangle)}{2E_0 - E_∞ e^{-2βE_∞} + \sqrt{\sinh^2(βΔ_g\langle σ \rangle) + e^{-2βE_∞}}}. \tag{19}
\]

In Fig. 3 we show the results for \( \sim \langle σ \rangle^2 \) as a function of temperature for the parameters given in (17) and (18). We have also plotted the measured intensity of an additional super-lattice peak, which is proportional to the square of the lattice dimerization. We have normalized the experimental data such that agreement is obtained in the low-temperature regime.

The comparison between theory and the data for CuGeO₃ does not lead to a determination of the frustration \( α \) but indicates closeness to a first-order phase transition, as can be deduced from the closeness of the experimental points in Fig. 3 to the critical curves where \( E_0 ≈ E_c(E_∞) \), compare Fig. 2(b).

VI. THERMODYNAMICS

The entropy \( S \) and the specific heat \( c_V \) are obtained from the free energy (3) via

\[
S = -\frac{∂F}{∂T}, \quad c_V = T\frac{∂S}{∂T}. \tag{20}
\]
In the disordered phase the entropy is (for $E_\infty = 0$) temperature independent with a value of $k_B \ln(2)/2$ per site, which is only half of the expected value for a spin 1/2 chain. This is due to the fact that we did neglect up to now the spin-degrees of freedom of the domain-walls. In Fig. 1 we present results for $c_V(T)$ for the parameters given by (17) and (18).

FIG. 4. Specific heat for different parameters as a function of temperature. (a): $E_\infty = 0$. (b): $2E_\infty = 0.3$ meV. The inset in graph (a) shows the experimental data of $c_V/T$ in units of $[\text{mJ}/\text{K}^2]$ versus $T$ ($10^{-2}\text{meV}/\text{K}^2$ corresponds to 5.24$m\text{J}/\text{gK}^2$).

For small soliton excitation energies the results are typically mean-field like. For values of $E_0$ approaching the limit of the second-order phase regime the specific heat is strongly enhanced near $T_{SP}$. It will diverge as the transition becomes first-order. Note that the specific heat is linear in temperature for $E_\infty \leq E_0 < E_c$, in the limit $T \to T_{SP}$ and that the jump in the specific heat diverges as $E_0 \to E_c$ like $(E_c - E_0)^{-1}$. Right at $E_0 = E_c$ the specific heat diverges like $(T_{SP} - T)^{-1/2}$. Note that a similar divergence $\sim (T_{SP} - T)^{-0.4}$ has been reported in an early measurement for CuGeO$_3$ though the exact value of the specific heat critical exponent for CuGeO$_3$ is still controversial (14).

In the inset of Fig. 4 we present the measured magnetic contribution to the specific heat of CuGeO$_3$. A straightforward comparison with the results of the mean-field theory is not possible since all the entropy of the effective Ising chain is released in a mean-field approach. This corresponds to half of the entropy of the spin chain. Experimentally, only $\sim 10\%$ of the magnetic entropy is released at $T_{SP}$, since the exchange constant $J \approx 160\text{K} \gg T_{SP}$ and the measured specific heat is consequently smaller in magnitude than our mean-field result. The neglect of the soliton dispersion relation (2) is, on a microscopic level, the reason for this discrepancy between theory and experiment. A qualitative comparison is nevertheless possible and favors an $E_0$ close to the first-order phase transition.

Up to know we did not take the spin-degree of freedom of the solitons into account, as they just contribute a constant factor to the partition function in the paramagnetic case. As we have no magnetic interactions between the spins of different solitons in our model we can evaluate the magnetic susceptibility simply by Curie’s law

$$\chi(T) = \frac{g^2 \mu_B^2 S(S + 1)}{3k_B T} n(T) \approx 1.16 \frac{\mu_B^2}{k_B T} n(T),$$

where $\mu_B = gJ/(2m,e)$ is the Bohr magneton, $g = 2.15$ the measured $g$-factor of the Cu$^{2+}$-ion, $S = 1/2$ and $n(T)$ the density of thermally activated solitons per site. $n(T)$ is obtained differentiating the free energy with respect to $E_s$:

$$n(T) = \frac{\partial F/L}{\partial E_s} = \frac{1}{2\lambda_0} \frac{e^{-2\beta E_s}}{\sqrt{\sinh^2(\beta \Delta g(\sigma)) + e^{-2\beta E_s}}}.$$

Above $T_{SP}$ this expression reduces to

$$n(T > T_{SP}) = \frac{1}{2 e^{2\beta E_\infty} + 1}.$$

The mean number of solitons attains 1/4 per site, as the temperature goes to infinity, corresponding to half a soliton per dimer. The results for the magnetic susceptibility are shown in Fig. 3. The fast drop of $\chi(T)$ below $T_{SP}$ for larger values of the soliton excitations energies is again reminiscent of the experimental data for CuGeO$_3$. Our susceptibility rises though much higher at $T_{SP}$ than the experimental data which is a direct consequence of the neglected soliton dispersion (4). In the limit of large temperatures $T \gg J$ the theoretical curve drops to 1/4 of the experimental points as a consequence of the aforementioned soliton density (23) (at 300K $\approx 2J$ it has dropped to about 1/2 of the magnitude of the experimental data).
Note that for the curves plotted as solid lines in Fig. 3, Fig. 4, and Fig. 5, which are closest to the experimental data within the parameters chosen by us, entropy, specific heat, and susceptibility are overestimated by about the same factor of five.

\[ 0 \leq T_0 = 0.277 \text{meV} \]
\[ 0 \leq T_0 = 0.2 \text{meV} \]
\[ 0 \leq T_0 = 0.1 \text{meV} \]
\[ 0 \leq T_0 = 0.0 \text{meV} \]
\[ E_{\infty} = 0.15 \text{meV} \]

FIG. 5. Magnetic susceptibility for different parameters as a function of temperature. (a): \( E_{\infty} = 0 \). (b): \( 2E_{\infty} = 0.3 \text{meV} \). The inset in graph (a) shows the experimental data of \( \chi \) in units of \( [10^{-9} \text{m}^3/\text{mole}] \) versus \( T \) (0.01\( \mu_B^2/k_B \)K correspond to 47.12 \( \cdot 10^{-9} \text{m}^3/\text{mole} \)).

VII. SINGLET–TRIPLET GAP

The gap to triplet excitations is given by Eq. (9),

\[ \Delta_N = 2 \left( E_{\infty} + (E_0 - E_{\infty})(\sigma)^2 \right) + c' J \left( \frac{\Delta_g(\sigma)}{J} \right)^{2/3}, \]

(24)

with \( c' = 2.33 \). A straightforward application of (24) would yield, compared with experiment, a much too large zero-temperature gap \( 2E_0 + c' J(\Delta_g/J)^{2/3} \). This is so since the order parameter \( \langle \sigma \rangle (T = 0) \) takes the value one in the molecular-field approximation, while it is much smaller than unity for CuGeO\(_3\). We have therefore decided to use the parameter \( c' \) in (24) to fix \( \Delta_N(T = 0) \) to the experimentally observed value 2.5meV. The results are given in Fig. 6, together with the measured gap for CuGeO\(_3\).

VIII. CONCLUSIONS

We have discussed a simple mean-field theory for spin-Peierls transitions applicable both for phonon-driven \( (\alpha < \alpha_c) \) and for magnetically driven \( (\alpha > \alpha_c) \) spin-Peierls transitions. We have applied the approach to CuGeO\(_3\) and found that it is not possible to determine uniquely from the experimentally measured temperature...
dependence of the order-parameter the magnitude of the frustration parameter $\alpha$.

The theory allows both for a first-order and a second-order spin-Peierls transition, depending on the parameters of the model. We find that the parameters which fit experiments best indicate that CuGeO$_3$ is close to a first-order phase transition.

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