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Pressure dependence and non-universal effects of microscopic couplings on the spin-Peierls transition in $CuGeO_3$

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Abstract. The theory by Cross and Fisher (CF) is by now commonly accepted for the description of the spin-Peierls transition within an adiabatic approach, involving however a continuum approximation for the relevant response function. Using density matrix renormalization group (DMRG) techniques we are able to treat the spin system *on the lattice* exactly up to numerical inaccuracies. Thus we find the correct dependence of the equation of state on the spin-spin interaction constant which in the CF theory drops out completely. With respect to $CuGeO_3$ we focus on the pressure dependence of the critical temperature and analyze the ratio of the spectral gap and the transition temperature.

PACS. 75.10.Jm Quantized spin models – 75.50.Ee Antiferromagnetics – 75.40.Cx Static properties (order parameter, static susceptibility, heat capacities, critical exponents, etc.)

1 Introduction

Low dimensional quantum systems are currently of considerable interest mainly due to the fascinating phase transitions driven by strong quantum fluctuations. The continuous interest from the theoretical side is provoked by the discovery of many experimental systems realizing quasi one-dimensional quantum systems. In the field of spin-Peierls systems the discovery of the inorganic compound $CuGeO_3$ realized a milestone as many measurements have been performed with high accuracy since. Therefore, $CuGeO_3$ has attracted much attention in experimental as well as in theoretical works. The high temperature behaviour of $CuGeO_3$ was found to be modelled adequately by one-dimensional frustrated Heisenberg chains [1–4]. In the dimerized phase, many features were shown to be consistent within an adiabatic description of the phonon degrees of freedom. This observation comprises zero temperature [5–8] as well as thermodynamic properties [2,4].

Even in one space dimension only a few exact results exist, particularly concerning thermodynamics. For integrable systems the thermodynamical potentials and asymptotic behaviour of correlation functions are known. A notorious problem is posed by response functions and non-integrable systems in general. With respect to this, the recently developed transfer matrix DMRG (TMRG) [9–11] on the basis of transfer matrices [12] provides a very powerful method to calculate thermodynamic quantities of spin chains without any use of perturbative methods. This has been demonstrated in several applications [4,11,13–17]. The first description of the spin-Peierls transition and thermodynamics beyond a continuum limit was given in [2] on the basis of exact diagonalization. The present TMRG method allows for a systematic enhancement with respect to finite size effects for the important low temperature regime [4].

In this paper we study the influence of microscopic coupling constants on the spin-Peierls transition temperature. This allows for an understanding of the considerable pressure dependence of the phase diagram along the following line of reasoning. It is known that external pressure affects the magnetic properties of $CuGeO_3$ considerably [3,18,19]. Fits for the magnetic susceptibility yield the change of the nearest-neighbour spin interaction J and estimates for the frustration parameter α. Using these data for J as function of pressure we are able to explain the observed increase of the spin-Peierls temperature and estimate the pressure dependence of the next-nearest-neighbour exchange.

The outline of the paper is as follows. In Section 2 we present the model and a motivation for our description of the experimentally studied spin-Peierls systems. We study the static dimerization susceptibility in Section 3. Section 4 is devoted to the computation of the critical temperature as a function of the spin exchange couplings and external pressure, respectively. We give a comparison of our results with experimental measurements. In Section 5 we investigate the spectral gap and its ratio to the spin-Peierls temperature. The conclusion is given in Section 6.

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2 Model

In the inorganic spin-Peierls compound $CuGeO_3$ the magnetic interactions are attributed to Heisenberg spin exchange. There is numerous evidence that in addition to the nearest-neighbour interaction (J) a next-nearest-neighbour exchange $J' = \alpha J$ [1–3] with $\alpha = 0.35$ has to be taken into account. Usually the constant α is referred to as frustration parameter.

At the spin-Peierls temperature the system undergoes a structural phase transition driven by the quantum spin system coupled to the phonons. The spin-phonon coupling is modelled by spin exchange integrals depending linearly on the local displacements. The adiabatic treatment yields a quantum spin system coupled to just one phonon mode with the commonly used Hamiltonian

$$\hat{H} = \sum_i \left\{ J\left[(1+\delta_i)\mathbf{S}_i\mathbf{S}_{i+1} + \alpha\mathbf{S}_i\mathbf{S}_{i+2}\right] + \frac{K}{2}\delta_i^2 \right\}, \quad (1)$$

where $\mathbf{S}_i$ are spin 1/2 operators, $\delta_i = (-1)^i\delta$ denotes the modulation of the magnetic exchange couplings in the dimerized phase. Here, we restrict ourselves to vanishing external magnetic field where the system shows a phase transition from the uniform (U), *i.e.* $\delta = 0$, to the dimerized (D) phase ($\delta > 0$).

The elastic energy can be expressed in terms of microscopic constants rendering (1) equivalent to an RPA treatment of the phonon propagator for the full spin-phonon system. Within RPA the condition for the phase transition is identical to that for (1) as formulated in (4) below if K is adjusted to the following value [20]

$$K = \frac{J^2}{2}\left(\sum_i \frac{\lambda_i^2}{M_i \Omega_i^2}\right)^{-1} =: \mathcal{C}J^2. \quad (2)$$

The sum runs over the spin-Peierls active modes. For each mode i, M_i denotes the effective mass of the unit cell, Ω_i the frequency of the spin-Peierls active phonon and λ_i the spin-phonon coupling constant. In particular, K is proportional to J^2. The constant $\mathcal{C}$ contains only the microscopic parameters of the underlying lattice.

Our numerical investigations do not improve over those of CF [21] with respect to the RPA treatment. However, within the RPA approximation we deal with the complete dynamics of the quantum spin system. Note that in reference [21] a continuum description of the spin system was used with a subsequent bosonization treatment which is believed to capture only the long distance asymptotics of the correlation functions.

3 Response functions

The static dimerization susceptibility of the spin system is defined by

$$A_\alpha(x) = -J^{-1} \lim_{\delta\to 0} \frac{\partial^2 f_\alpha(x,\delta)}{\partial\delta^2}, \quad (3)$$

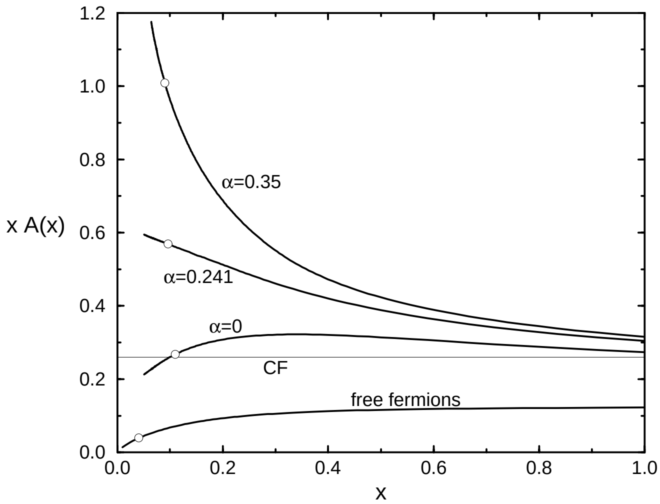

Fig. 1. Depiction of the function $xA(x)$ with $x = T/J$ for: free fermions, Heisenberg model in continuum limit (CF), and TMRG results for frustration parameter $\alpha = 0, 0.241, 0.35$. The circles denote the relevant values for $CuGeO_3$ (see text).

where $x = T/J$, and $f_\alpha(x,\delta)$ is the free energy per site for system (1) with fixed dimerization δ, frustration α and K set to zero. The response function A is nothing but the correlation of the nearest neighbour spin exchange $\mathbf{S}_i\mathbf{S}_{i+1}$ (dimer operator) at momentum $q = \pi$ and energy $\omega = 0$. The U/D phase transition takes place for

$$A_\alpha(x_{\mathrm{SP}}) = K/J = \mathcal{C}J. \quad (4)$$

For details the reader is referred to [4].

Let us now review the results obtained by CF. Within the bosonization approach they find $xA_{\alpha=0}(x) = \chi_0$ with $\chi_0 \approx 0.26$. As a direct consequence by use of the inversion of (4),

$$T_{\mathrm{SP}} = JA_\alpha^{-1}(\mathcal{C}J), \quad (5)$$

this yields $\mathrm{d}T_{\mathrm{SP}}/\mathrm{d}J = 0$. Of course, this is also clear from the fact that the energy scale of the spin system completely drops out due to scale invariance.

Figure 1 shows a comparison of our TMRG results[1] for the function $xA_\alpha(x)$ for various values of α with the findings of CF and exact data for free fermions. The enormous progress achieved by the numerical analysis is the correct treatment of the spin system on the lattice at practically all length scales. This improves over the continuum limit approach in which the asymptotics of correlation functions is incorrectly extended to short distances. For the unfrustrated Heisenberg model, *i.e.* $\alpha = 0$, we are able to observe directly the deviations between the continuum limit and a lattice treatment of the spin degrees of freedom.

With respect to $CuGeO_3$ we fix J by the requirement that the experimental magnetic susceptibility equals

[1] We have used 24 states in the renormalization step and have set the accuracy with respect to Trotter decomposition to $(TM)^{-1} = 0.05$.

that of the strictly one-dimensional model *at* the critical point leading to $J = 130K$ ($\alpha = 0$), $J = 150K$ ($\alpha \approx \alpha_c \approx 0.2412$ [1,22,23]), $J = 160K$ ($\alpha = 0.35$), and $J = 350K$ (free fermions). The circles in Figure 1 denote the values of $xA_\alpha(x)$ at the experimentally determined spin-Peierls temperature $T^0_{\rm SP} = 14.4$ K for $CuGeO_3$ (see *e.g.* [24–26]). These values imply constants (*cf.* Eq. (4)) $\mathcal{C}_0 \approx 0.019\ {\rm K}^{-1}$ ($\alpha = 0$), $\mathcal{C}_{0.241} \approx 0.040\ {\rm K}^{-1}$ ($\alpha = 0.241$), $\mathcal{C}_{0.35} \approx 0.070\ {\rm K}^{-1}$ ($\alpha = 0.35$), and $\mathcal{C}_{\rm ff} \approx 0.0027\ {\rm K}^{-1}$ (free fermions).

For the unfrustrated model the value $x_{\rm SP}A_{\alpha=0}(x_{\rm SP})$ almost coincides with the results of CF. However the agreement happens only fortuitously since χ_0 is a zero temperature quantity. For other frustration parameters qualitative and quantitative deviations from the CF-line appear. The divergence of $A(x)$ for free fermions, Heisenberg model with $\alpha < \alpha_c$, $\alpha = \alpha_c$, and $\alpha > \alpha_c$, is $\log(x)$, $1/x \times$ log. corrections [4,27], $1/x$ (see [22] and references therein), and exponential [4], respectively. The quantitative values for $x_{\rm SP}A(x_{\rm SP})$ also differ from each other. We must conclude that it is risky to deduce quantitative results from the bosonization approach as already pointed out by CF. For applications to $CuGeO_3$ it is furthermore uncertain if the pure Heisenberg chain can even yield the qualitative results correctly. From the analysis of the susceptibility data at higher temperature we are led to favour the frustration parameter $\alpha = 0.35$ [2–4] for which the behaviour of the response function deviates considerably from χ_0/x.

4 Pressure dependence of the magnetic system

From (5) it is straightforward to deduce the dependence of the spin-Peierls temperature on the variation of the spin coupling constants. The relation is valid for every fixed value of α. We first focus on the system with $\alpha_0 = 0.35$ at ambient pressure.

The dependence of J and α on the external hydrostatic pressure have already been obtained from the relation between magnetostriction and the pressure dependence of the magnetic susceptibility χ [3]. From our TMRG data we find $\frac{\partial\chi}{\partial \ln J} \gg \frac{\partial\chi}{\partial \ln \alpha}$ at constant temperature. These two quantities appear in the following expression, $\frac{{\rm d}\chi}{{\rm d}p} = \sum_i \frac{\partial\chi}{\partial \ln x_i}\frac{\partial \ln x_i}{\partial p}$, where $x_1 = J$ and $x_2 = \alpha$. Therefore, we conclude the value for the pressure dependence of J to be more reliable than that of α. The authors of reference [3] deduced a value of $\frac{{\rm d}\ln J}{{\rm d}p} = -7.0(5)\%/{\rm GPa}$ using the relation between magnetostriction and pressure dependences of J and α. Using in addition the experimentally determined value for the pressure dependence of the spin-Peierls temperature $\frac{{\rm d}T_{\rm SP}}{{\rm d}p} \approx 4.8$ K/GPa [18] we obtain the relation $T_{\rm SP}(J)$ (thick black line in Fig. 2).

Due to the particular geometry involved in the superexchange mechanism we expect the magnetic exchange energies to respond much more sensitively to the pressure (bond-bending mechanism [28,29]) than the phonon frequencies or the spin-phonon coupling constants. We therefore consider $\mathcal{C}$ as independent of pressure which applicability for $CuGeO_3$ will break down at higher pressure. The numerical results with $\mathcal{C} = \mathcal{C}_{0.35}$ are shown in Figure 2. Obviously, a constant value of $\alpha = 0.35$ (dashed-dotted line) can not explain the observed behaviour, even yielding a change of the critical temperature to opposite direction.

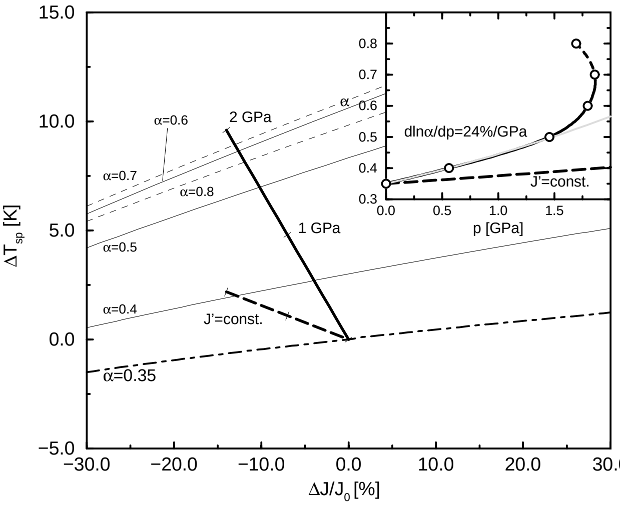

Fig. 2. Variation of the spin-Peierls temperature *versus* the relative change of the magnetic exchange coupling. The lines show TMRG results for constant α and fixed $\mathcal{C}_{0.35}$. The thick black line displays the experimental behaviour as an implicit function of pressure. The dashed (dashed-dotted) line shows the theoretical results for ${\rm d}J'/{\rm d}p = 0$ (${\rm d}\alpha/{\rm d}p = 0$). The corresponding dependences of α on the pressure are shown in the inset.

From geometrical reasons we expect J' to be non-decreasing. Assuming $J' =$ constant to be realized, the increase of $T_{\rm SP}$ is too small by a factor of approximately 4 (as displayed by the thick dashed line in Fig. 2). Consequentially, the main effect must be a strong increase of J'. The deduced dependence of α on the hydrostatic pressure fits well with $\frac{{\rm d}\ln\alpha}{{\rm d}p} = 24 \pm 2\%/{\rm GPa}$ (or $\frac{{\rm d}\ln J'}{{\rm d}p} = 17 \pm 2\%/{\rm GPa}$ respectively) up to about 1.4 GPa as displayed in the inset of Figure 2. The error was determined assuming that the value of $\frac{{\rm d}T_{\rm SP}}{{\rm d}p}$ involves an error of ± 0.5 K/GPa, where the uncertainty in $\frac{{\rm d}\ln J}{{\rm d}p}$ only plays a secondary role. In general, already the weak requirement that J is non-increasing with hydrostatic pressure gives a minimum pressure dependence of $\frac{{\rm d}\ln\alpha}{{\rm d}p} \geq 20\%/{\rm GPa}$. The pressure dependence of α has already been investigated in reference [3], however, with large error bounds which are respected by our results. The divergence of $\frac{{\rm d}\ln\alpha}{{\rm d}p}$ at a finite pressure or in other words, an upper limit of the critical temperature, is a physical prediction of the chosen one-dimensional approach. It is mostly based on a limited spontaneous gap as a function of α. But as already mentioned above, we expect an agreement with $CuGeO_3$ only in the low pressure region.

Table 1. Pressure dependences of the spin system parameters and the spin-Peierls temperature as explained in the text. Numbers in bold face denote results obtained by our DMRG calculations, all other quantities were used as input data. Note that models based on free fermions or unfrustrated Heisenberg chains can not explain the rather large pressure dependence of the critical temperature.

	$\frac{\mathrm{d}\ln J}{\mathrm{d}p}$[%/GPa]	$\frac{\mathrm{d}\ln\alpha}{\mathrm{d}p}$[%/GPa]	$\frac{\mathrm{d}T_{\mathrm{SP}}}{\mathrm{d}p}$[K/GPa]
free fermions	≈ -6	(0)	$\approx$**1.8**
$\alpha = 0$	≈ -5	(0)	$\approx$**0.3**
$\alpha_0 = 0.35$	-7.0 ± 0.4	**24±2**	4.8 ± 0.5

A similar analysis can be done on the basis of the unfrustrated Heisenberg model and free fermions. Evaluating the magnetic susceptibility data of Takahashi *et al.* [18] we derive $\frac{\mathrm{d}\ln J}{\mathrm{d}p} \approx -5\%/\mathrm{GPa}$ ($\alpha = 0$) and $\frac{\mathrm{d}\ln J}{\mathrm{d}p} \approx -6\%/\mathrm{GPa}$ (free fermions). In contrast to the frustrated case, a change of α under pressure for these initially unfrustrated models is not reasonable. The deduced theoretical decrease of the critical temperature is too small by a factor of about 3 for free fermions (or equivalently Hartree-Fock calculations), in the case of the unfrustrated Heisenberg model even by a factor of ≈ 15 (see Tab. 1).

We must conclude that neither the unfrustrated Heisenberg model nor Hartree-Fock results are able to describe the physics of $CuGeO_3$ correctly. In contrast to this a Heisenberg model with parameters $\alpha_0 = 0.35$ and $\frac{\mathrm{d}\ln\alpha}{\mathrm{d}p} = 24\%/\mathrm{GPa}$ turns out to reproduce the experimental findings up to about 1.4 GPa.

5 "BCS-ratio"

Another interesting quantity is the ratio of the singlet-triplet gap to the spin-Peierls temperature, known as "BCS-ratio". Combining the TMRG data for A with zero temperature DRMG calculations for the singlet-triplet gap as a function of α and the dimerization one gets a relation between Δ_{ST} and T_{SP}. The results are shown in the bottom section of Figure 3.

Using the scaling of A [4], the definition of the critical temperature and the dependence of the ground state energy on small saturation dimerizations $\delta_0 = \delta(T = 0)$ one finds

$$\delta_0 \simeq {T_{\mathrm{SP}}}^{3/2} \exp(-\frac{\Delta^0_{\mathrm{ST}}}{2}/T_{\mathrm{SP}}), \tag{6}$$

ignoring logarithmic corrections for $\alpha < \alpha_{\mathrm{c}}$. Here Δ^0_{ST} denotes the singlet-triplet gap for vanishing dimerization, which is zero for $\alpha \leq \alpha_{\mathrm{c}}$. In the next step we apply $\Delta_{\mathrm{ST}} - \Delta^0_{\mathrm{ST}} \simeq \delta_0^{2/3}$ [30,31] to derive an explicit asymptotic relation between the gap and the spin-Peierls temperature,

$$\Delta_{\mathrm{ST}} - \Delta^0_{\mathrm{ST}} \simeq T_{\mathrm{SP}} \exp(-\frac{\Delta^0_{\mathrm{ST}}}{3}/T_{\mathrm{SP}}), \tag{7}$$

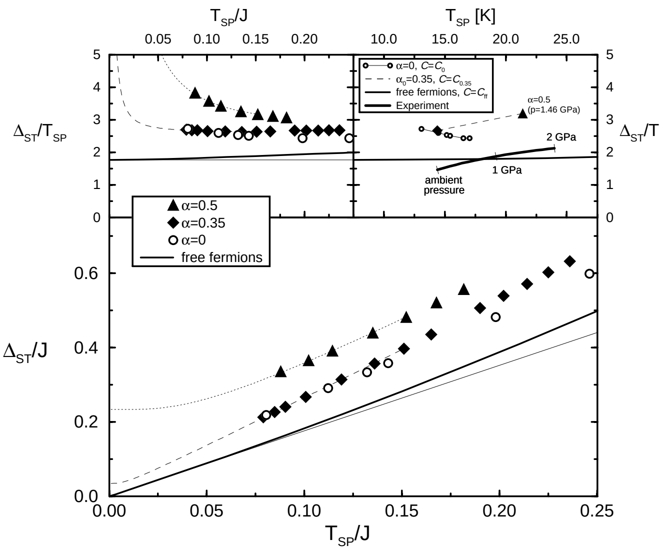

Fig. 3. Bottom: Singlet-triplet gap Δ_{ST} as a function of the spin-Peierls temperature. Symbols denote the DMRG results, the solid line shows the exact result for free fermions. The thin lines show the expected behaviour from the scaling of A (see text). Top left: Ratio of the spin gap and spin-Peierls temperature ("BCS ratio"). Top right: "BCS ratio", experiment *versus* theory.

again neglecting logarithmic corrections for $\alpha < \alpha_{\mathrm{c}}$. The thin lines in Figure 3 show fits according to equation (7) in the range up to $T/J = 0.15$. For $\alpha = 0.5$ we used the known value $\Delta^0_{\mathrm{ST}} = 0.2338J$ [32,33], hence only performed a one-parameter fit in the presented region. For $\alpha = 0.35$ a spontaneous gap of $\Delta^0_{\mathrm{ST}} = 0.035J$ is used, also derived by $T = 0$ DMRG. For $\alpha = 0$ the predicted linear behaviour (*cf.* (7)) can not be seen due to the logarithmic corrections. A linear extrapolation of our data points shows a positive offset. However, this is consistent with the presence of logarithmic corrections since we expect a zero limit at $T = 0$ with infinite slope. The free fermions show the well known behaviour $\Delta_{\mathrm{ST}}/T_{\mathrm{SP}} \approx 1.76$. We now derive the "BCS-ratio" as a function of the spin-Peierls temperature simply by dividing by T_{SP} (upper left of Fig. 3). Firstly we observe that the Heisenberg like models have a distinctly larger "BCS-ratio" than free fermions.

For comparison to experiment we again fix the constant $\mathcal{C}$. Furthermore, the pressure dependence of J and the frustration derived in Section 4 is taken into account here. The results are shown in the top right of Figure 3. Interestingly, the experimental result [18] compares well with the low temperature asymptotics for free fermions but showing a pronounced increase with pressure which is not reproduced. From the investigations in reference [4] we already know for Heisenberg models that the gap and therefore the "BCS-ratio" is larger than the experimentally observed one. This happens due to the strictly one-dimensional treatment of $CuGeO_3$, *i.e.* the neglect of the dispersion perpendicular to the chain, which will lower the true gap. The unfrustrated chain even yields a qualitatively incorrect tendency of a decreasing "BCS-ratio" under pressure the appropriately frustrated system is at least able to explain the increase.

6 Conclusion

The TMRG analysis of the spin-Peierls phase transition allows a complete treatment of the quantum dynamics. In contrast to continuum descriptions correlations are respected at all length scales, which leads to the exact response functions. Within the scope of an adiabatic description, equivalent to RPA as in the CF theory, we are able to study the influence of the spin-spin exchange energy scale J on the critical temperature. We like to emphasize that these results are a non-trivial improvement over the CF theory which shows no dependence on J at all. Moreover, frustrated models can be investigated as well.

Using the pressure dependence of J it is possible to study the dependence of the spin-Peierls temperature on pressure. Neither Hartree-Fock calculations nor the unfrustrated Heisenberg chain yield the strong increase as measured. Once again, our investigations favour a frustration of $\alpha = 0.35$ for $CuGeO_3$ at ambient pressure. We find a rather strong dependence of the frustration on pressure, $\frac{\mathrm{d}\ln\alpha}{\mathrm{d}p} = 24\pm 2\%/\mathrm{GPa}$, which agrees with earlier studies [3].

The analysis of the "BCS-ratio" also gives a clear indication that frustration is present in $CuGeO_3$, even though some quantitative deviations can only be explained by residual perpendicular couplings. There is evidence for a strong dependence of α on pressure from the "BCS-ratio".

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