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Solitons in the spin-Peierls compound $CuGeO_3$

A.S.T. Pires[a]

Universidade Federal de Minas Gerais, Departamento de Física, CP 702, 30123-970, Belo Horizonte, MG, Brazil

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Abstract. We calculate the excitation gap, the soliton energy, and the soliton density at finite temperature, of the spin-1/2 one dimensional antiferromagnet coupled to phonons, using a self-consistent harmonic approximation, and the thermal-Green function technique. The spin degrees of freedom are represented by the phase Hamiltonian with the help of the boson representation of the spinless fermions. We estimate the critical field H_c above which begins the incommensurate phase. We also present a theoretical calculation for the specific heat in this phase. We use $CuGeO_3$ as an example of a compound where our theory could be applied.

PACS. 75.10.Jm Quantized spin models – 75.50.Ee Antiferromagnetics

1 Introduction

The spin-Peierls (SP) transition occurs in a system of one-dimensional quantum spin 1/2 antiferromagnetic chains coupled to three-dimensional phonons. At low temperatures it leads to dimerization of the lattice and formation of a gap in the spin excitation spectrum [1–5]. Interest in models of spins interacting with phonons has increased significantly since the identification of the first inorganic compound of this type, namely $CuGeO_3$ [4]. Pure $CuGeO_3$ has a SP transition at a temperature, T_{sp}, slightly above 14 K. Below T_{sp}, the system is in a dimerized spin singlet state, and the gap to the lowest triplet excitation is $\Delta = 23$ K. One of the features of the SP system is the possibility of applying a strong enough magnetic field to cancel the gap. This induces a transition to a new magnetic phase in which the periodicity of the spin-polarization and the associated lattice deformation is incommensurate with the underlying crystallographic lattice. This non-uniform state is in the form of a soliton lattice [5,6].

In the one dimensional $S = 1/2$ Heisenberg antiferromagnet, it is known that the quantum fluctuations drive the system into a liquid singlet ground state. This ground state is non-degenerate but critical, *i.e.* small perturbations may drive it magnetic (alternating fields) or shorter ranged resonating-valence-bond (RVB) type (external dimerization). In fact, as shown by Liang *et al.* [7] the Néel state and the RVB concept are different sides of the same medal. A technique very suited to treat the existence of the large quantum fluctuations in this system is the phase Hamiltonian. In this approach the original Hamiltonian is transformed to a fermionic Hamiltonian using the Jordan-Wigner transformation, and the fermionic model is bosonized [8]. The resulting continuum Hamiltonian is [8–11]

$$H = \int \mathrm{d}x \left[A \left(\frac{\mathrm{d}\theta}{\mathrm{d}x} \right)^2 - 2AQ \frac{\mathrm{d}\theta}{\mathrm{d}x} + Cp^2 - B \frac{u(x)}{u_0} \sin\theta(x) - D\cos 2\theta(x) + \frac{2K}{a} u(x)^2 - F\cos\theta(x) + \frac{F}{2} \langle \cos\theta(x) \rangle \right] \tag{1}$$

where $A = Ja/8$, $B = J\lambda u_0/a^2$, $C = \pi^2 Ja/2$, $D = \pi^2 J/8a$, $F = z|J'|\langle\cos\theta(x)\rangle/a$, $Q = g\mu_B H/4\pi A$; a, u_0, and λ denote the lattice constant, the staggered lattice displacement, and the spin phonon coupling constant respectively. The second term in equation (1) represents the Zeeman energy. The fourth term gives the contribution to the energy of the fermion system which is due to the lattice distortion, allowing for a spatially varying dimerization order parameter $u(x)$. The fifth term is due to umklapp scattering. The sixth term represents the energy associated with the lattice distortion. K is the elastic constant. The last two terms represent the weak interchain exchange interaction between the nearest neighbor chains, taken into account in a mean field approximation, and where z is the number of the nearest neighbor chains. The detailed calculation of equation (1) can be found in references [8–11]. Before going further, let us observe that the Hamiltonian (1) treats the phonon adiabatically, *i.e.* the lattice distortions are considered as static. For a discussion of phonon dynamics and the adiabatic approximation see reference [12].

Varying equation (1) with respect to $u(x)$ we obtain

$$(4K/a)u(x) - B\sin\theta(x) = 0. \tag{2}$$

[a] e-mail: antpires@fisica.ufmg.br

For $H = 0$, $J' = 0$, the solution $\theta = \pi/2$, $u(x) = u_0$ leads to the lowest energy to (1), which describes then the double sine-Gordon model. From the quantum point of view this equation can be treated as the usual quantum sine-Gordon equation [13]. Its spectrum consists of solitons, antisolitons and breathers, all with the same gap (equal to the magnon gap). The soliton corresponds to an excitation with $S^z = +1$, the antisoliton with $S^z = -1$, and the breather, $S^z = 0$. The soliton, the antisoliton and the lowest energy breather thus form the low-energy degenerate triplet excitation: the magnon. An applied magnetic field splits this triplet into its three components. In this section we consider the solution $\theta = \pi/2$, and calculate the quantum fluctuations intrinsic to the problem. In the next section we will study the case of a spatially varying $u(x)$.

In the method of Nakano and Fukuyama [9] the non-harmonic terms in equation (1) are treated, at $T = 0$ K, using the self-consistent harmonic approximation (SCHA) proposed by Dashen, Hasslacher and Neveu [14]. In the present paper, we extend the $T = 0$ K calculations performed by several authors [9–11,15] to finite temperatures. Within the SCHA the Hamiltonian (1) with $H = 0$ is transformed into [9–13]

$$\begin{aligned} H_{\mathrm{SCHA}} = \int \mathrm{d}x \Bigg[& A(\mathrm{d}\hat{\theta}/\mathrm{d}x)^2 + A(\mathrm{d}\theta_s/\mathrm{d}x)^2 + Cp^2 \\ & + \left(\frac{\widetilde{B}}{2}\frac{u(x)}{u_0}\sin\theta_s + 2\widetilde{D}\cos 2\theta_s + \frac{F}{2}\mathrm{e}^{\langle\theta^2\rangle/2}\cos\theta_s \right)\hat{\theta}^2 \\ & + \widetilde{B}\frac{u(x)}{u_0}\sin\theta_s \left(1 + \langle\hat{\theta}^2\rangle/2\right) - \widetilde{D}\cos 2\theta_s(1 + 2\langle\hat{\theta}^2\rangle \\ & - \frac{F}{2}\mathrm{e}^{-\langle\hat{\theta}^2\rangle/2}\cos\theta_s \left(1 + \langle\hat{\theta}^2\rangle\right) + \frac{2K}{a}u^2(x)\Bigg] \\ & + \int \mathrm{d}x \Bigg[2A\left(\frac{\mathrm{d}\theta_s}{\mathrm{d}x}\right)\left(\frac{\mathrm{d}\hat{\theta}}{\mathrm{d}x}\right) \\ & + \left(-\widetilde{B}\frac{u(x)}{u_0}\cos\theta_s + 2\widetilde{D}\sin 2\theta_s + F\mathrm{e}^{-\langle\hat{\theta}^2\rangle/2}\sin\theta_s \right)\hat{\theta}\Bigg], \end{aligned} \tag{3}$$

where $\langle\hat{\theta}^2\rangle$ is the self-consistent average of the fluctuations of the phase variable $\theta(x)$ around its classical value θ_s, and

$$\widetilde{B} = B\mathrm{e}^{-\langle\hat{\theta}^2\rangle/2}, \quad \widetilde{D} = D\mathrm{e}^{-2\langle\hat{\theta}^2\rangle}, \tag{4}$$

$$\widetilde{F} = \frac{z|J'|}{a}\mathrm{e}^{-\langle\hat{\theta}^2\rangle/2}\cos\theta_s. \tag{5}$$

For the ground-state, $u(x) = u_0$ and θ_s is a constant. The excitation spectrum corresponding to uniform θ is

$$\omega(q) = v\left(q^2 + q_0^2\right)^{1/2}, \tag{6}$$

where

$$q_0^2 = \frac{\widetilde{B}}{2A}\sin\theta_s + \frac{2\widetilde{D}}{A}\cos 2\theta_s + \frac{F}{2A}\mathrm{e}^{-\langle\hat{\theta}^2\rangle}\cos\theta_s, \tag{7}$$

and v is the spin wave velocity $v = 2\sqrt{AC} = Ja\pi/2$. For the harmonic Hamiltonian $\langle\hat{\theta}^2\rangle$ is given by

$$\langle\hat{\theta}^2\rangle = \frac{C}{L}\sum_q \frac{1}{\omega(q)} = \frac{C}{\pi}\int_0^\pi \frac{\mathrm{d}q}{\omega(q)}, \tag{8}$$

where L is the length of the chain. The finite-temperature effect is handled in terms of the thermal Green's function. In this approach we take [16]

$$\frac{1}{\omega(q)} \to \sum_n \frac{T}{\omega_n^2 + \omega(q)}, \tag{9}$$

or

$$\langle\hat{\theta}^2\rangle = \frac{C}{\pi}\int_0^\pi \frac{\mathrm{d}q}{\omega(q)}\coth\left(\frac{1}{2}\beta\omega(q)\right), \tag{10}$$

which can be written as

$$\langle\theta^2\rangle = \frac{C}{\pi}\int_0^\pi \frac{\mathrm{d}q}{\omega(q)} + 2CF_0, \tag{11}$$

where

$$F_0 = \frac{1}{\pi}\int_0^\pi \frac{\mathrm{d}q}{\omega(q)}\frac{1}{\mathrm{e}^{\omega(q)/T} - 1}\cdot \tag{12}$$

At $T = 0$ K we have $\langle\hat{\theta}^2\rangle = \ln(2\pi/aq_0)$, where we have assumed $q_0 \ll \pi$.

The ground state of the Hamiltonian (1), in the absence of the magnetic field, is the spin-Peierls (SP) state or the Néel state.The SP state corresponds to $\theta_s = \pi/2$, while in the Néel state we have $\theta_s = 0$.

(1) *The spin-Peierls state*

Substituting $\theta_s = \pi/2$ into equation (7) gives

$$q_0^2 = \left(\widetilde{B}/2 - 2\widetilde{D}\right)/A. \tag{13}$$

This state coincides with the one studied by Nakano and Fukuyama [9] because the interchain exchange interaction does not contribute to the SP state since it has no magnetic moment. The ground state is non-magnetic and defined by the quantum number $S = 0$, where S is the total spin operator. The excitations given by equation (6) represent a band of triplet excitations separated from the ground state by the gap $\Delta = \omega(0) = vq_0$. These magnon-like excitations are usually characterized as the elementary excitations of the SP system. However, it should be made clear that the excitations are not spin wave Goldstone modes, but triplets, *i.e.* they are three-fold degenerate.

From equation (13) we obtain at $T = 0$ K, $q_0 = \pi(2\delta/3\pi)^{2/3}$, where $\delta = \lambda u_0/a^2$ is the bond alternation induced by lattice dimerization, the result obtained in reference [9]. For $CuGeO_3$, if we take the values given by Castilla *et al.* [2], $J = 150$ K, $\delta = 0.03$, we find $\Delta = 23.6$ K, in reasonable agreement with the experimental value [4] $\Delta \approx 23$ K. Let us now consider the

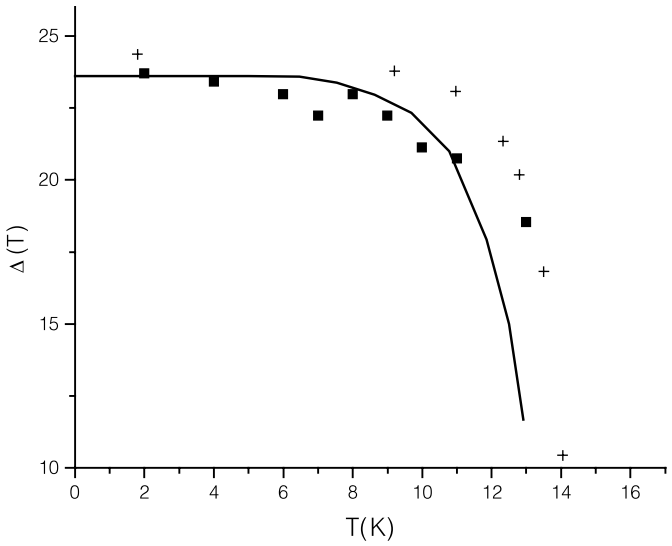

Fig. 1. Energy gap, $\Delta = vq_0$, as a function of temperature for $J = 150$ K and $\delta = 0.03$. (We have used the temperature dependence of the parameter δ given in Ref. [18].) Experimental data from reference [19] are indicated with solid squares, and experimental data from reference [20] are indicated with crosses.

effect of a non zero temperature. In the theory we use here the lattice displacement, u_0, is an input parameter, and our theory gives a temperature dependence for the gap Δ even if u_0 is taken as a constant. However, for $CuGeO_3$, u_0 has an intrinsic temperature dependence. In fact, it is the vanishing of this parameter with temperature that leads to the spin-Peierls transition. It is not our purpose here the calculation of $u_0(T)$ but mainly the temperature dependence of the critical field, once $u_0(T)$ is known. To the best of our knowledge there is no theoretical calculation of $u_0(T)$, although near T_{sp} a Landau Theory can be used [17]. However, Riera and Dobry [18] have calculated $\delta(T) = \lambda u_0(T)/a^2$ numerically, and hence we can use their temperature dependence (scaled to our value of δ at $T = 0$ K) in our calculations. In Figure 1 we display the energy gap as a function of temperature for $J = 150$ K and $\delta = 0.03$, using this temperature dependence for $\delta(T)$. In this figure we also show the experimental data from references [19] and [20]. The reasonable agreement, between our theoretical calculation and the experimental data, is an indication that the procedure we have adopted here works, at least at low temperatures.

(2) *The Néel state*

Substituting $\theta_s = 0$ into equation (7) gives

$$q_0^2 = \frac{2\widetilde{D}}{A} + \frac{F}{2A}\mathrm{e}^{-\langle\hat{\theta}^2\rangle}. \tag{14}$$

Comparing the ground-state energies between dimerized phase and the AFM phase we get that the crossover from $\theta_s = \pi/2$ to $\theta_s = 0$ is determined by [10]

$$r = J\lambda^2\left(\sqrt{3}z\gamma K a^2\right)^{-1}, \tag{15}$$

where $\gamma = J'/J$. If $r > 1$ the system is dimerized; otherwise the ground state has long-range antiferromagnetic order. For the $CuGeO_3$ we find that the condition for the SP state is $\gamma < 0.1$, which is consistent with the fact that this compound is dimerized at zero temperature.

2 Soliton formation energy

A soliton (*i.e.* a spatially varying $u(x)$) is a possible solution besides the uniform solution $u(x) = u_0$ examined in the previous section. In zero magnetic field, the soliton solution has lower energy than the spin-triplet excitation with the gap Δ. Solitons, at $T = 0$ K, have been studied in the literature [9–11,15] and we refer the reader to these articles for further details. In this section we are interested in solitons at finite temperatures. As a starting point we present the soliton solution. We will assume that $\langle\hat{\theta}^2\rangle$ is uniform in space, even though $\theta_s(x)$ varies spatially, and is given by equation (9). Thus there will be no spatially varying renormalized parameter in our equation. One consequence of this assumption is that the magnetic (ξ_m) and the distortive (ξ_d) soliton widths are identical. However, the results in reference [5] shed some doubt on this equality. Taking into account the spatial dependence of the renormalizing factors $\exp(-\langle\hat{\theta}^2\rangle/2)$ and $\exp(-2\langle\hat{\theta}^2\rangle)$ could explain the experimentally observed difference between (ξ_m) and (ξ_d) [5]. In fact, a fully self-consistent numerical calculation [21] gives $\xi_d/\xi_m = 1.24$. We intend, in the future, to take into account the spatial dependence of $\langle\hat{\theta}^2\rangle$.

We will require that $\theta_s(x)$ satisfies the following differential equation so that the first order term in in equation (2) vanishes:

$$2A\left(\frac{\mathrm{d}\theta_s}{\mathrm{d}x^2}\right) + \widetilde{B}\frac{u(x)}{u_0}\cos\theta_s - 2\widetilde{D}\sin 2\theta_s - F\mathrm{e}^{-\langle\hat{\theta}^2\rangle/2}\sin\theta_s = 0. \tag{16}$$

Minimization of the energy with respect to the variations of $u(x)$ and $F(x)$ leads to equation (2) with the substitution $B \to \widetilde{B}$, and to

$$F(x) = zJ'\mathrm{e}^{-\langle\hat{\theta}^2\rangle/2}\cos\theta_s/a. \tag{17}$$

From equations (15, 16) and (17) we obtain

$$\frac{\mathrm{d}\theta_s}{\mathrm{d}x^2} - \frac{1}{2\xi^2}\sin 2\theta_s = 0, \tag{18}$$

where

$$\frac{1}{\xi^2} = q_0^2 - \frac{4\gamma z}{a^2}\mathrm{e}^{-\langle\hat{\theta}^2\rangle}. \tag{19}$$

From equation (19) we can see that the soliton width is increased substantially by the interchain coupling. In this section we will consider $J' = 0$, and soliton solutions of the form

$$\cos\theta_s = \pm\tanh(x/\xi). \tag{20}$$

This soliton excitation, although with an energy lower than the spin-wave gap, has spin $S = 1/2$, and therefore it can not be excited by a neutron. If topological solitons exist in the spin-phonon model such excitations should be created in pairs. In the 1D spin-phonon model solitons and anti-solitons are not bound in pairs. However, when the interchain elastic coupling, $K_\perp$ is taken into account, a bound state in the isolated chain appear to become a more defined coherent excitation. Dobry and Ibaceta [22] have studied the formation of solitonic structures in spin-Peierls systems including the three-dimensional character of the phonon field using the SCHA at $T = 0$ K. They consider then a pair of solitons. As the chain gets decoupled ($K_\perp \to 0$) the energy of the pair is twice the creation energy of a soliton in the single chain problem. When the interchain coupling is switched on they show that it is more favorable to create a domain (bound-pair) rather to excite a magnon. This result lead them to identify the low-energy resonance as due to a domain excitation. A bound state is a triplet excitation because its total S^z could be 0 or ± 1, and it has formation energy smaller than the magnon gap. (Magnetic internal excitations of the domain would give further excitations of the system.) This interpretation seems to be more adequate. As we will see the soliton energy is inversely proportional to the soliton width ξ, and as we have seen the interchain coupling J' enhances ξ, and thus reduces the observed gap value for a given dimerization δ. This result is consistent with a number of recent investigations [5].

To calculate the formation energy of a soliton, in the dimerized phase, at finite temperature it is necessary to calculate the thermodynamic potential of the soliton sector given by $\Omega_S = \Omega - \Omega_0$, where Ω is the thermodynamical potential in the presence of a soliton and Ω_0 is the one in the absence of the soliton. We have

$$\Omega_S = E_S^0 + \Omega_B + \Omega_{cont} + \widetilde{E}, \tag{21}$$

where $E_S^0 = E_C + E_{elas}$, E_c is the classical soliton energy, and E_{elas} is the change in the elastic energy. The second and third terms in the right hand side of equation (21) correspond to the thermodynamical potential of a gas of bosons (phasons) given by

$$\Omega_B = T\left\{\ln[2\sinh(\omega_B/2T)] - \ln[2\sinh(\omega(0)/2T)]\right\}, \tag{22}$$

$$\begin{aligned}\Omega_{cont} &= T\sum_{q\neq 0}\left\{\ln[2\sinh(\omega(q)/2T)] - \ln[2\sinh(\omega(k)/2T)]\right\} \\ &= \frac{T}{\pi}\int_0^\Lambda \mathrm{d}k\delta(k)\left[\frac{\mathrm{d}}{\mathrm{d}k}\ln[2\sinh(\omega(k)/2T)]\right].\end{aligned} \tag{23}$$

where ω_B is the frequency of the bound state (that appears in the presence of a soliton) given by [9] $\omega_B = \omega(0)(\sqrt{3}/2)^{1/2}$, and $\omega(q)$ and $\omega(k)$ are the frequencies in the presence and in the absence of a soliton, respectively. Here $\delta(k)$ is the phase shift of the $\theta(x)$ field with wave number k scattered by the static soliton. Finally, $\widetilde{E}$ is given by [9]:

$$\widetilde{E} = C\langle\theta^2\rangle(2\pi\xi)^{-2}, \tag{24}$$

with $\langle\theta^2\rangle$ given by equation (9). Integrating equation (23) by parts we find

$$\begin{aligned}\Omega_{cont} = \frac{T}{\pi}\Bigg\{&\delta(k)\ln[2\sinh(\omega(k)/2T)]\Big|_\infty \\ &- \delta(0)\ln[2\sinh(\omega(0)/2T)] \\ &- \int_0^\Lambda \ln[2\sinh(\omega(k)/2T)]\frac{\mathrm{d}\delta}{\mathrm{d}k}\mathrm{d}k\Bigg\}.\end{aligned} \tag{25}$$

The phase shift is given by [9]

$$\delta(k) = \arg\frac{\Gamma\left(1-\mathrm{i}\widetilde{k}\right)\Gamma\left(-\mathrm{i}\widetilde{k}\right)}{\Gamma\left(-\mathrm{i}\widetilde{k}-s\right)\Gamma\left(-\mathrm{i}\widetilde{k}+s+1\right)}, \tag{26}$$

where here $\widetilde{k} = k/q_0$, $s = (\sqrt{3}-1)/2$, and $\Gamma(z)$ is the gamma function. We can show that:

$$\delta(0) = -\pi/2, \quad \text{and for} \quad k\to\infty \quad \delta(k) = -s(s+1)/\widetilde{k}.$$

After some algebra we arrive at the following result

$$\frac{\mathrm{d}\delta}{\mathrm{d}k} = \frac{1}{q_0}\frac{\mathrm{d}\delta}{\mathrm{d}\widetilde{k}}, \tag{27}$$

where

$$\begin{aligned}\frac{\mathrm{d}\delta}{\mathrm{d}\widetilde{k}} = \frac{s}{s^2+\widetilde{k}^2} + \sum_{n=0}^{\infty}\Bigg[&\frac{2(1+n)}{(1+n)^2+\widetilde{k}^2} \\ &-\frac{1+s+n}{(1+s+n)^2+\widetilde{k}^2} - \frac{1-s+n}{(1-s+n)^2+\widetilde{k}^2}\Bigg].\end{aligned} \tag{28}$$

For the pure sine-Gordon model we have $s = 1$ and the sum in equation (28) is easily performed leading to the result

$$\frac{\mathrm{d}\delta}{\mathrm{d}k} = \frac{2}{1+\widetilde{k}^2}\cdot \tag{29}$$

Now to proceed we use the relation

$$T\ln[2\sinh(\omega/2T)] = \omega/2 + T\ln\left(1-\mathrm{e}^{-\omega/T}\right), \tag{30}$$

so that we can write

$$\begin{aligned}\Omega_S = E_S + T\ln\left(1-\mathrm{e}^{-\omega_B/T}\right) - \frac{T}{2}\ln\left(1-\mathrm{e}^{-\omega(0)/T}\right) \\ + \omega^2(0)F_0 - TF_2,\end{aligned} \tag{31}$$

where

$$F_2 = \frac{1}{\pi}\int_0^{\pi} \ln\left(1 - \mathrm{e}^{-\omega(k)/T}\right)\frac{\mathrm{d}\delta}{\mathrm{d}k}\mathrm{d}k. \tag{32}$$

and

$$E_S = \left[\frac{1}{\pi} + \frac{1}{2}\left(\frac{\sqrt{3}}{2}\right)^{1/2} - \frac{1}{4} - \frac{1}{4\pi} - \frac{1}{2\pi}\int_0^{\pi} \mathrm{d}k\sqrt{1+\widetilde{k}^2}\frac{\mathrm{d}\delta}{\mathrm{d}\widetilde{k}}\right]\omega(0). \tag{33}$$

The integral in equation (33) has to be evaluated numerically. The result $E_S = 0.3119\omega(0)$ was obtained in reference [9]. However, if we replace $\widetilde{k}$ by $\sin\widetilde{k}$ in the integral in equation (33) (which is more appropriate in a discrete lattice), we find $E_S = 0.3913\omega(0)$.

At finite temperatures, we can extract the soliton energy from Ω_S by

$$E_S(T) = \Omega_S - T\left(\frac{\mathrm{d}\Omega_S}{\mathrm{d}T}\right). \tag{34}$$

We have to take into account the temperature dependence of the gap $\omega(0)$ when we carry out the total derivative $(\mathrm{d}\Omega_S/\mathrm{d}T)$ in equation (34). Up to the leading order in the coupling constant this term cancels exactly the term arising from $\partial\Omega_S/\partial T$. Writing

$$E_S(T) = E(0) + \Delta E(T), \tag{35}$$

we have

$$\Delta E(T) = \frac{\omega_B}{\mathrm{e}^{\omega_B/T}-1} - \frac{1}{2}\frac{\omega(0)}{\mathrm{e}^{\omega(0)/T}-1} + \frac{1}{\pi}\int_0^{\pi}\frac{\mathrm{d}k}{\mathrm{e}^{\omega(k)/T}-1}\left[\frac{\omega^2(0)}{\omega(k)} - \omega(k)\frac{\mathrm{d}\delta}{\mathrm{d}k}\right]. \tag{36}$$

In the numerical evaluation of equation (36) we have to take into account the temperature dependence of q_0.

In the dimerized phase of a spin-Peierls system solitons can be excited thermally or induced by disorder. The role played by solitons excitations in the description of the SP transition was considered, in a qualitative way, in reference [23]. The authors have shown that solitons could strongly affect the properties of spin-Peierls systems even at $H = 0$, and in their approach the phase transition occurs at a temperature when the thermally excited soliton-antisoliton pairs dissociate. From the thermodynamic potential the soliton density of thermally excited solitons can be calculated [24] and it reads

$$n_S = \frac{(E_S/2)}{\pi^{3/2}v}\mathrm{e}^{-\beta\Omega_S}. \tag{37}$$

From equation (37) several thermodynamic quantities can be obtained.

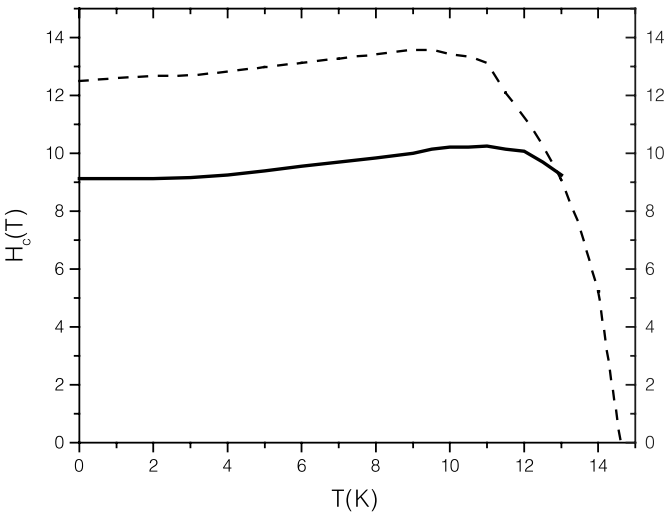

Fig. 2. Critical field H_c, above which begins the incommensurate phase, as a function of the temperature. The dashed line represents the D-I phase transition obtained experimentally by Boucher and Regnault [1].

In the presence of a magnetic field the energy of the SP state remains unchanged as far as the state in nonmagnetic [11], but the formation energy of a soliton is field dependent and is given by

$$E_S(H) = E_S - g\mu_B H/2. \tag{38}$$

The critical field, H_c, for the spontaneous formation of solitons, and an occurrence of a commensurate-incommensurate transition, is given by $E_S(H) \approx 0$, *i.e.* $H_c = 2E_S/g\mu_B$. The incommensurate state is in the form of a soliton lattice, and it has a non zero magnetization. At $T = 0$ K, using the calculation of Nakano and Fukuyama [9] for the soliton energy, we have $H_c = 0.624\Delta/g\mu_B$. The modified integral (using $k \to \sin k$) gives $H_c = 0.78\Delta/g\mu_B$, while the experimental value is [4] $H_c = 0.84\Delta/g\mu_B$. In view of the ambiguity in the numerical constants used in the continuum-limit calculations, the obtained theoretical values should be considered as estimates. In Figure 2 we show H_c as a function of temperature for the same values of the parameters used in Figure 1. We have used $E_S(0)$ as calculated in reference [9]. We also show the D-I phase transition line obtained experimentally by Boucher and Regnault [1] and Palme *et al.* [25] (the line *I*-*U*, where *U* means the uniform phase, is not shown in the figure). We could get a better agreement using the calculation for a discrete lattice, but given the uncertainty in the parameters (theoretical and experimental) this could be fortuitous. If we consider the parameter δ as a constant the soliton energy, and therefore the critical field, increases monotonically with the temperature. This behavior is in contrast with the pure sine-Gordon model where the soliton energy decreases with temperature. We can trace this difference of behavior mainly to the first term in equation (36) which is absent in the pure sine-Gordon model, since in this case the bound state energy is zero. If we take $\delta(T)$ temperature

dependent, with the temperature dependence given in reference [18], the final result is that the critical field exhibits a smooth maximum. This behavior, for the critical field, has been obtained before phenomenologically by Bulaevskii *et al.* [26] and Buzdin *et al.* [27], and is in agreement with the experimental data of references [1] and [25].

3 Incommensurate phase

As we have mentioned in the last section for fields stronger than some critical field H_c, spin-solitons are spontaneously formed, and we have an incommensurate (IC) phase. Inagaki and Fukuyama [11] have studied this phase using a semi-SCHA approach. In this section we consider quantum fluctuations, neglected in reference [11], added to the classical Hamiltonian. For the IC phase the spatial variation of $\theta(x)$ or the displacement $u(x)$ is essential. We start with the Hamiltonian written in the following form

$$\begin{aligned} H = A\int \mathrm{d}x \Bigg\{ & \left(\frac{\mathrm{d}\hat{\theta}}{\mathrm{d}x}\right)^2 + \frac{C}{A}p^2 \\ & + \frac{2\pi^2}{a^2}\left[\widetilde{\eta} + \widetilde{j}' + (-\widetilde{\eta} + 2\widetilde{d} + \widetilde{j}')\cos 2\theta_s\right]\hat{\theta}^2 \\ & + \left(\frac{\mathrm{d}\theta_s}{\mathrm{d}x}\right) - 2Q\frac{\mathrm{d}\theta}{\mathrm{d}x} - \frac{2\pi^2}{a^2}\left[(\widetilde{\eta} + \widetilde{j}')(1 + \langle\hat{\theta}^2\rangle)\right] \\ & + \frac{2\pi^2}{a^2}\left[(\widetilde{\eta} - \widetilde{j}')(1 + \langle\hat{\theta}^2\rangle) - \widetilde{d}(1 + 2\langle\hat{\theta}^2\rangle)\right]\cos 2\theta_s \Bigg\}, \end{aligned} \tag{39}$$

where, following reference [11] we have defined

$$\begin{aligned} & \eta = J\lambda^2/4\pi^2 K a^2, \quad j' = zJ'/\pi^2 J \\ & \widetilde{\eta} = \eta \mathrm{e}^{-\langle\hat{\theta}^2\rangle}, \quad \widetilde{j}' = j'\mathrm{e}^{-\langle\hat{\theta}^2\rangle}, \quad \widetilde{d} = \mathrm{e}^{-2\langle\hat{\theta}^2\rangle}/2. \end{aligned} \tag{40}$$

In general, the solution of the sine-Gordon equation are regularly spaced solitons, a "soliton lattice", given in terms of elliptic functions [28]. The sine-Gordon equation can be put in the form

$$\frac{\mathrm{d}x}{\mathrm{d}\theta} = \frac{1}{\sqrt{b^2 + 4\gamma^2\sin^2(\theta/2)}}, \tag{41}$$

where $\gamma^2 = (4\pi^2/a^2)[(\widetilde{\eta} - \widetilde{j}')(1 + \langle\hat{\theta}^2\rangle) - \widetilde{d}(1 + 2 + \langle\hat{\theta}^2\rangle)]$, and b^2 is a constant. The periodic solution of equation (40) is $\cos\theta = sn(\gamma x/\sqrt{m}, m)$, where $m = 4\gamma^2/(b^2 + 4\gamma^2)$. Substituting equation (41) into equation (39) we obtain for the soliton energy in the incommensurate phase, and at $T = 0$ K, the following expression

$$\frac{E}{A} = \frac{4\gamma E(m)}{\sqrt{m}} - 2\pi Q - \frac{\gamma^2}{2}\left(1 + \frac{b^2}{2\gamma^2}\right)d, \tag{42}$$

where d is the soliton spacing given by $d = 2\sqrt{m}K(m)/\gamma$, and $K(m)$ and $E(m)$ are the complete elliptic integrals of the first and second kind. Minimizing (41) with respect to b^2, and using

$$\frac{\mathrm{d}}{\mathrm{d}b^2}\left(\frac{4\gamma E(m)}{\sqrt{m}}\right) = \frac{d}{4}, \tag{43}$$

we obtain $E(m)/\sqrt{m} = 2\pi Q/4\gamma$. The energy of the commensurate (dimerized) phase is [11]

$$\frac{E_c}{d} = \frac{v}{4\pi}\left(\frac{\pi}{a}\right)^2 - \frac{4\pi^2}{3a^2}A\eta^2. \tag{44}$$

The incommensurate phase is more stable than the dimerized phase for $Q > Q_c$, where Q_c is given by $2\pi Q_c = 4\gamma$. The critical field of the commensurate-incommensurate transition is then

$$g\mu_B H_c = \frac{4}{3\pi}\omega(0)\sqrt{1 + \frac{1}{2}\langle\hat{\theta}^2\rangle - \frac{3}{2}(1 + \langle\hat{\theta}^2\rangle)\frac{j'}{\eta}}. \tag{45}$$

If we take $\delta = 0.03$, we have $q_0 = 0.2158$ and $\langle\hat{\theta}^2\rangle = \ln(2\pi/q_0) = 3.37$, which, for $J' = 0$, leads to $g\mu_B H_c = 0.728\ \omega(0)$. This value compares reasonably with the one obtained in the former section, while it differs from the value $g\mu_B H_c = 0.424\ \omega(0)$ calculated in [11].

We now investigate the small oscillations of a soliton lattice. Let

$$\theta(x,t) = \theta_s(x) + \vartheta(x)\mathrm{e}^{-\omega t}. \tag{46}$$

Taking (46) into equation (18) and linearizing with respect to ϑ we obtain a Lamé's equation which was solved in references [29–33]. In the extended-zone scheme, the spectrum consists of two branches, the first lying inside the first Brillouin zone and the second lying outside. The spectrum has only a single gap, occurring at the edge of the first zone $q = \pm q_m = \pm\pi/d$. In the long-wavelength limit $q \ll q_m$, the dispersion relation, for a three dimensional system, reported in reference [30] is

$$\omega^2(q) = c_x^2 q_x^2 + c_y^2 q_y^2 + c_z^2 F(m) q^2, \tag{47}$$

where

$$F(m) = \sqrt{m'}K(m)/E(m), \quad \text{with} \quad m' = 1 - m. \tag{48}$$

Fetter and Stephen [30] have shown that equation (48) is quite an accurate representation for all $|q| \ll q_m$. Taking $k_x = c_x q_x$, $k_y = c_y q_y$, $k_z = vFq_z$, as well as $x = k/k_B T$, we obtain for the energy

$$U = \frac{(k_B T)^4}{(c_x c_y v F)}\frac{1}{(2\pi)^2}\int_0^\infty \frac{x^3 \mathrm{d}x}{\mathrm{e}^x - 1}, \tag{49}$$

which gives the following expression for the specific heat

$$C_P = \beta_m T^3, \tag{50}$$

with

$$\beta_m = \frac{\pi^2}{15}\frac{k_B^3}{(c_x c_y v F)}\,. \tag{51}$$

Hence the "phasons" give rise to a T^3 contribution in the specific heat, which is indeed experimentally observed [3,5]. This T^3 behavior of the specific heat in the

incommensurate phase has been predicted previously on general grounds in the literature [17,34], but here we obtain this behavior from an specific microscopic model. If we knew the values of the parameters c_x and c_y appearing in equation (47) we could obtain the explicit value of the coefficient β_m in equation (50) and compare with the experimental value [3] $\beta_m = 1.4\ \mathrm{mJ\,mole^{-1}\,K^{-4}}$. The value of C_P, given by equation (50), does not strongly change as a function of the magnetic field. This result is also in agreement with the experiments.

We remark that although the sine-Gordon equation, in the IC phase, has been intensively studied in connection with superconductors [29–31], most of the results have not, as yet, being applied to the SP problem.

4 Conclusions

We have performed analytical calculations of the excitation gap and the soliton energy, at finite temperature, of a spin Peierls system using the phase Hamiltonian and the SCHA. We have calculated the temperature dependence of the critical field for the spontaneous formation of solitons; *i.e.* the transition between the commensurate and incommensurate phases. In addition, we have presented a calculation for the specific heat in the IC phase, and commented about some points that could be useful to a better understanding of the SP problem.

To compare the theoretical calculations with the experiments we have chosen $J = 150$ K, and $\delta = 0.03$. This set of parameters was given by Castilla *et al.* [2] and gave the best fit to the value of the gap. However, other values have being reported in the literature. The discrepancy in the several set of parameters came from differing emphasis in the fitting procedures. Given the ambiguity in the numerical constants used in the continuum limit calculation and the several set of parameters (J, J', δ) reported in the literature we conclude that more work needed to be done to a better understanding of $CuGeO_3$. As we have mentioned briefly in Section 2, even the nature of the gap is not well settled.

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