Magnetostriction in an array of spin chains under magnetic field

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We consider an array of XX spin-1/2 chains coupled to acoustic phonons and placed in a magnetic field. Treating the phonons in the mean field approximation, we show that this system presents a first order transition as a function of the magnetic field between a partially magnetized distorted state and the fully polarized undistorted state at low temperature. This behavior results from the magnetostriction of the coupled chain system. A dip in the elastic constant of the material near the saturation field along with an anomaly in the magnetic susceptibility is predicted. We also predict the contraction of the material as the magnetic field is reduced (positive magnetostriction) and the reciprocal effect i.e. a decrease of magnetization under applied pressure. At higher temperature, the first order transition is replaced by a crossover. However, the anomalies in the susceptibilities in the system near the saturation field are still present. We discuss the relevance of our analysis in relation to recent experiments on spin-1/2 chain and ladder materials in high magnetic fields.

I. INTRODUCTION

The subject of Bose-Einstein Condensation (BEC) has become tremendously active both experimentally and theoretically in the recent years due to the observation of BEC in trapped atomic gases. Another way of obtaining a BEC, predicted theoretically some time ago, is to place a quasi one dimensional spin gap systems under a strong magnetic field, causing the formation of a Luttinger liquid of magnons. This Luttinger liquid possesses a quasi-long range order, which is a one dimensional precursor of the BEC. In the presence of any three dimensional coupling, this quasi-condensed state develops a long-range order, which corresponds to a BEC of the magnons. This condensation has been observed experimentally in spin-1 chain materials, and more recently in Cu$_2$(C$_5$H$_{12}$N$_2$)$_2$Cl$_4$ (CuHpCl), a material originally believed on the basis of its thermodynamics to be formed of weakly coupled two leg ladders. However, it is now known that CuHpCl is in fact formed of dimers coupled in a three-dimensional network, and that the Bose condensation is a condensation of a two or three-dimensional magnon Bose fluid. Recently, such a Bose-Einstein condensation of magnons has also been observed in other coupled dimers systems such as TiCuCl$_2$, KCuCl$_2$, Cs$_3$Cr$_2$Br$_6$ and BaCu$_2$Si$_2$O$_6$. Theoretical description taking into account the two-dimensional nature of these gapped systems have been developed in recent years. They are based on the bond operator theory (BOT) description of the coupled dimer system. The interactions between the condensed triplet bosons are treated by the Hartree-Fock-Popov (HFP) approximation, and a rigid lattice is assumed. However, more recently, some experimental evidence for a lattice distortion associated with the Bose Einstein Condensation has been obtained. Older reports of specific heat anomalies also pointed out to a lattice distortion associated with the transition. It has thus been suggested that the distortion observed in experiments could be the generalized spin-Peierls transition predicted originally for spin ladder systems under field. However, similarly to the conventional spin-Peierls transition, in a generalized spin-Peierls transition the lattice distortion results from an optical phonon becoming static. As a result, in the generalized spin-Peierls transition, the lattice constants of the crystal do not change, but superlattice peaks are visible in X-Ray diffraction, in contrast with experiments. In fact, in the case of a condensate of magnetic excitations coupled to a deformable lattice, another instability than the generalized spin-Peierls transition is possible, namely magnetostriction. Although magnetostriction has been mostly discussed in the context of ferromagnetism, it can also be observed in paramagnetic or antiferromagnetic systems. In the case of magnetostriction, the lattice parameters change as the system becomes magnetized, but the number of atoms per unit cell does not change, which means that no new reflection appear in X-Ray diffraction experiments. In a ferromagnet, magnetostriction is known to turn the second order Curie transition into a first order transition. Thus, the magnetostrictive effects may also explain the first order transition as a function of magnetic field observed in magnon Bose-Einstein condensation experiments. Besides the Bose-Einstein condensation of magnons in spin gap systems, magnetostriction effects are also relevant near the saturation field in the spin-1/2 chain material Cu(II)-2,5bis(pyrazol-1-yl)-1,4-dihydroxybenzene (CuCCP). In fact, the two effects can be closely related as a ladder system under strong magnetic field can be mapped for strong rung coupling on an anisotropic spin-1/2 chain. In the present paper, we will discuss a model of magnetostriction in 1D XX spin chains coupled by 3D acoustic phonons.
We will study the effect of phonon coupling at the mean field level and show that the Bose Einstein Condensation transition of the magnons becomes a first order transition at low temperature. The origin of the first order character of the transition can be traced to the hardcore repulsion of the magnons, which prevents the collapse of the condensate. Treatments based on Hartree-Fock-Popov mean field theory neglect the hardcore constraint and thus fail in the regime where the first order transition is obtained. This stresses that a correct treatment of the hardcore constraint is necessary to describe the first order transition observed in experiments.

The plan of the paper is the following. In Sec. III we introduce a model of an array of two leg ladders coupled with classical phonons as a minimal model to describe the BEC in a system of hard core bosons coupled to a lattice deformation. From this model we deduce an effective XXZ spin chain Hamiltonian that can be rewritten in terms of a free fermion Hamiltonian by the Jordan-Wigner transformation. In Sec. III we focus on the zero temperature case. By a mean field theory, we discuss the first order phase transition at varying the external magnetic field and the pressure. In particular, we derive a Ginzburg-Landau expansion of the free energy valid for a very stiff lattice which allows an analytical discussion of the behavior of the magnetization and of the lattice parameter as a function of the magnetic field. We also calculate and discuss the behavior of various susceptibilities in the distorted case, such as the elastic modulus, the magnetic susceptibility and the magnetostriction coefficient that all present anomalies at the transition.

In Sec. IV we turn to the positive temperature case and deduce first a Ginzburg-Landau expansion which allows us to predict the temperature above which the first order transition is replaced by a crossover. All the susceptibilities are then recalculated at finite temperature and some results compared to recent experiments. We also consider the behavior of the dilatation coefficient and of the specific heat. Finally in Sec. V we give the conclusions and perspectives for future work.

II. MODEL

In order to grasp the origin of the first order character of the BEC in a spin gap system under field coupled to acoustic phonons, we want to build a model that can be solved with a minimum of approximation. We will start with an array of two leg ladders coupled with classical phonons. Its Hamiltonian reads:

\[ H = \sum_{n,m} \left( 1 + \eta (u_{n,m} - u_{n+1,m}) \right) \left[ J_\parallel (S_{n,m}^x S_{n+1,m}^x + S_{n,m}^y S_{n+1,m}^y) + J_\perp S_{n,m}^z S_{n+1,m}^z \right] + J_\perp \sum_{n,m} S_{n,2m} \cdot S_{n,2m+1} + \frac{K}{2} (u_{n,m} - u_{n+1,m}) \]

where \( J_\parallel, J_\perp > 0 \) are the exchange constants, \( K \) is the elastic constant, and \( \eta \) is a spin-phonon coupling constant. We have neglected the kinetic energy of the phonons, as is done usually in treatments of magnetostriction. In the case of a strong rung interaction \( J_\perp \), it is possible to reduce the size of the Hilbert space by considering only the singlet rung state and the triplet state of spin \( S^z = +1 \) and derive an effective XXZ spin chain theory. The resulting effective Hamiltonian reads:

\[ H = J_\parallel \sum_{n,m} \left( 1 + \delta_{n,m} \right) \left( T_{n,m}^x T_{n+1,m}^x + T_{n,m}^y T_{n+1,m}^y + \Delta T_{n,m}^z T_{n+1,m}^z \right) + \frac{K}{2} S_{n,m}^2 - h' T_{n,m}^z, \]

where the pseudospin operator is acting on the reduced Hilbert space, \( \delta_{n,m} = \eta (u_{n+1,2m} - u_{n,2m}) \) (we are assuming \( u_{n+1,2m} - u_{n,2m} = u_{n+1,2m+1} - u_{n,2m+1} \) as we are only considering magnetostriction effects), \( K = K/\eta^2, \Delta = J_{\parallel}^2/(2J_{\parallel}) \), and \( h' = H - J_\perp - J_{\parallel}^2/2 \) is an effective magnetic field. The magnetization per rung of the ladder system is \( \bar{m} = \left\langle \left( S_{n,2m}^z + S_{n,2m+1}^z \right) \right\rangle = \left\langle T_{n,m}^z \right\rangle + 1/2 \). In the case of \( SU(2) \) invariant spin ladders \( J_\parallel = J_{\parallel}^2 \), one recovers \( \Delta = 1/2 \). The case of CuC CP is also described by the model defined by Eq. (2) with \( \Delta = 1 \) and the magnetization given by \( \left\langle T_{n,m}^z \right\rangle \). It is interesting to note that the operators \( T_{n,m}^\pm = (T_{n,m}^x \pm i T_{n,m}^y) \) satisfy the same commutation relation as hardcore boson creation and annihilation operators. As a result, the Hamiltonian also describes a system of hard-core bosons with nearest neighbor repulsion and a boson-phonon interaction. The magnetic field \( h' \) plays the role of the chemical potential of the hardcore bosons. When \( h' \) is sufficiently negative, the density of bosons is zero. In the original problem described by Eq. (1) this corresponds to the spin gap state obtained for \( H \ll J_\perp \). When \( h' \) is less negative, the density of hardcore bosons in the ground state becomes nonzero. As our system is one-dimensional, this leads to the formation of a quasi-Bose condensate of hard-core bosons, in which the order parameter of the Bose condensation \( T_{n,m}^\pm \) possesses quasi-long range order in the ground state. Hence, the transition between the spin gap state and the magnetized state in coupled dimer systems can be viewed as the Bose condensation of hard core triplet bosons. In the case we are considering, we have to consider the effect of the phonons on this Bose condensation. Let us first show that the HFP approximation can be inadequate to deal with the magnetostriction effects resulting from
the spin-phonon interaction\textsuperscript{49}. Indeed, if we consider bosons with an on-site repulsion described by the Hamiltonian:

\[ H = \sum_{\langle i,j \rangle} \left[ -t(1 + \delta_{ij})b_i^\dagger b_j + \frac{K}{2} \delta_{ij}^2 \right] - \mu \sum_i b_i^\dagger b_i + U \sum_i b_i^\dagger b_i(2b_i^\dagger b_i - 1) + V \sum_{\langle i,j \rangle} b_i^\dagger b_ib_j^\dagger b_j, \tag{3} \]

we notice that in one dimension and in the limit \( U \to \infty \), the Hamiltonian (3) becomes equivalent to the Hamiltonian (2) with \( J = t/2 \), \( V = J\delta \), and \( \mu = h' \). Let us make the HFP approximation \( b_i \to \langle b_i \rangle = \lambda \), \( \delta_{ij} \to \delta \) in (3). The resulting ground state energy reads:

\[
E = N \left[ -zt(1 + \delta)\lambda^2 - (\mu + U)\lambda^2 + (U + zV)\lambda^4 + \frac{K}{2} \delta^2 \right],
\]

\[
= N \left[ -(\mu + U + zt)\lambda^2 + \left( U + zV - \frac{z^2\lambda^2}{2K} \right) \left( \lambda^4 - \frac{\mu + U + zt}{2(U + zV - \frac{z^2\lambda^2}{2K})} \right) + \frac{K}{2} \left( \delta - \frac{zt}{K} \lambda^2 \right)^2 \right] + Ct, \tag{4}
\]

where \( z \) is the coordination number of the lattice. For \( U + zV - \frac{z^2\lambda^2}{2K} > 0 \), the variational energy Eq. (4) is bounded from below, and the minimization of (4) leads to:

\[
\lambda^2 = \frac{\mu + U + zt}{2U + 2zV - \frac{z^2\lambda^2}{2K}} \Theta(\mu + U + zt), \tag{5}
\]

\[
\delta = \frac{zt}{K} \frac{\mu + U + zt}{2U + 2zV - \frac{z^2\lambda^2}{2K}} \Theta(\mu + U + zt), \tag{6}
\]

where \( \Theta(x) \) is the Heaviside step function. From Eqs. (5)–(6), we obtain a second order phase transition as \( \mu > \mu_{\text{c}}^{(\text{HFP})} = -zt - U \). For \( U + zV - \frac{z^2\lambda^2}{2K} < 0 \), the variational energy (4) becomes unbounded from below. In that case, the HFP approximation leads to an unphysical result \( |\lambda| = \infty \). The origin of this unphysical behavior when the spin-phonon interaction becomes too strong is easily seen. The HFP approximation reduces the spin-phonon coupling to an effective attractive interaction between the bosons of order \( t^2/K \), and when this attraction overcomes the repulsion \( U + zV \), the ground state of the mean-field Hamiltonian becomes ill-defined. It is possible to propose an \textit{ad hoc} modification of the HFP approximation that takes into account the hard-core constraint. In the limit \( U \to \infty \), one must have \( b_i^\dagger b_i \leq 1 \). This constraint can be satisfied by imposing \( |\lambda|^2 \leq 1 \) on the order parameter and using as the variational energy Eq. (4) with \( U = 0 \). Then, one obtains that for \( zV - \frac{z^2\lambda^2}{2K} < 0 \), there is a first order transition, with \( \lambda = 0 \) and \( \delta = 0 \) for \( \mu < -zt + zV - t^2/(2K) \) and \( \lambda = 1 \) and \( \delta = zt/K \) for \( \mu > -zt + zV - t^2/(2K) \). The modified HFP approximation suggests that first-order magnetostrictive transition caused by the condensation of triplet excitations can be observed also in \( d > 1 \) provided the spin-phonon interaction is strong enough. The preceding discussion suggests that in order to describe correctly the first order magnetostrictive transition associated with the Bose condensation of the triplets, we need to treat exactly the hardcore interaction of the triplets. In the quasi-one dimensional system of Eq. (2), this can be done in principle exactly thanks to the integrability of the XXZ spin chain\textsuperscript{50}. The mean field theory of the magnetostrictive transition then proceeds\textsuperscript{48} by writing \( \delta_{n,m} = \delta \Theta(n, m) \) and minimizing the free energy with respect to \( \delta \). The parameter \( \delta \) measures the relative change of the lattice parameter \( \delta \propto \Delta a/a \). In the most general case, the free energy of the general XXZ chain in the presence of magnetostriction have to be obtained from the Thermodynamic Bethe Ansatz (TBA)\textsuperscript{43,52,53,54}. However, given the complexity of the TBA equations, it is better to consider the simplest case of \( \Delta = 0 \) i.e. \( J_\parallel = 0 \) (XX chain) as in the original theory of the spin-Peierls transition\textsuperscript{38,55}. In that particular case, by the Jordan-Wigner (JW) transformation\textsuperscript{56}:

\[
T_n^+ = a_n^+ \cos \left( \pi \sum_{m < n} a_m^+ a_m \right), \tag{7}
\]

\[
T_n^- = a_n^+ a_n - 1/2, \tag{8}
\]

the chain can be mapped to a chain of free fermions and the calculation of its thermodynamics is much simplified. We expect that this mapping is not going to affect the qualitative properties of the chain under field. In fact, when the magnetization per site of the XXZ chain is near saturation, i.e. when the density of triplet excitations created on the ladders is low, the effect of the short range interaction measured by \( \Delta \) becomes small. This is seen in particular in the behavior of the Luttinger exponent \( K \) which goes to 1 in that low density limit\textsuperscript{57}. Thus, we expect that the magnetostrictive effects that happen near the transition between the singlet state and the polarized state will be properly described by the model (2) with \( \Delta = 0 \). However, for a quantitative approach to the full magnetization
curve, the use of TBA equations would become necessary. Even then, the insight gained from the study of the XX chain will be useful to devise the correct treatment of the TBA equations combined with the self-consistency condition on $\delta$. Returning to the XX chain, after the JW transformation, and going to Fourier space, the Hamiltonian of the chain reads:

$$H = -J(1-\delta) \sum_k \cos ka_k^\dagger a_k + \frac{K}{2} \delta^2 - h(a_k^\dagger a_k - 1/2)$$

(9)

where we have written $J = J_\parallel$ and $h = h'$ to simplify the notation. The operator $a_k$ annihilates a fermion of momentum $k$. To study the thermodynamics, we consider that the system is under fixed pressure, and work with the Gibbs free energy. The variational Gibbs free energy reads:

$$G(p, T, h; \delta) = K \delta^2 + p\delta + \frac{h}{2} - T \int_{-\pi}^{\pi} \frac{dk}{2\pi} \ln(1 + e^{-((1-\delta)\epsilon(k)-h)/T})$$

(10)

where $P$ is the pressure, $p = \eta P$ is the reduced pressure and we have units in which $\hbar/k_B = 1$. The value of $\delta$ is obtained by minimizing $G(p, T, h; \delta)$ with respect to $\delta$. This yields the equation:

$$K\delta(p, T, h) + p = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\epsilon(k)}{e^{((1-\delta)\epsilon(k)-h)/T} + 1}$$

(11)

and the Gibbs free energy is then $G(p, T, h) = G(p, T, h; \delta(p, T, h))$. In the following sections, we will study the Eq. (11) at zero temperature, and exhibit the first-order magnetostrictive transition as a function of the applied field. We will also discuss the effect of the magnetostrictive effects on various susceptibilities of the system. Then, we will turn to the effect of a positive temperature.

### III. ZERO TEMPERATURE

In this section, we first show that at $T = 0$ and within mean field theory, a first order phase transition as a function of the external magnetic field is obtained in the array of 1D XX chain coupled to acoustic phonons. Then, using a Landau-Ginzburg expansion, valid in the case of a stiff lattice, we obtain analytically the expression of the discontinuity in the magnetization and in the lattice parameter. This allows us to represent the hysteresis cycle of the magnetization as a function of the applied magnetic field. Finally, we discuss the anomalies in the elastic constant and the magnetic susceptibility near the transition as well as the magnetostriction coefficient.

#### A. Minimization of enthalpy at zero temperature

##### 1. First order transition

In order to study the equilibrium value of the relative change in the lattice parameter $\delta$, we need an expression of the Gibbs free energy as a function of $\delta$ valid for $T = 0$. At zero temperature, the Gibbs free energy reduces to the enthalpy $H(p, h; \delta) = E_0(h; \delta) + p\delta$, where $E_0$ is the ground state energy. The ground state of the Hamiltonian is simply the Fermi sea of pseudofermions filled up to the chemical potential $h$. The Fermi wavevector of pseudofermions is given by $-J(1-\delta) \cos k_F = h$, and the magnetization $M = \langle T^z \rangle$ can be expressed as a function of $k_F$ as:

$$M = \frac{k_F}{\pi} - \frac{1}{2}.$$  

(12)

Using the magnetization $M$ instead of the Fermi wavevector, we can rewrite the ground state of the system as:

$$E(M, h, \delta) = -\frac{J}{\pi}(1-\delta)\cos(\pi M) + \frac{K}{2} \delta^2 - hM$$

(13)

The enthalpy must be minimized with respect to $\delta$ for fixed $h, p$ giving:

$$K\delta + p + \frac{J}{\pi} \cos(\pi M) = 0,$$

(14)
which is the zero temperature limit of Eq. (11), and the magnetization is given by:

$$J(1 - \delta) \sin \pi M - h = 0.$$  \hspace{1cm} (15)

Both Eqs. (14) - (16) are valid only for $|M| < 1/2$. For $M = \pm 1/2$, the kinetic energy of the pseudofermions vanishes, and $E_0 = K \delta^2/2 - hM$. In this saturated regime, one has obviously $\delta = -p/K$ independent of the magnetization.

In the regime of non-saturated magnetization, $\delta$ varies with the magnetization and the magnetic field, implying the existence of magnetostrictive effects. For $|M| < 1/2$, it is possible to use the equation (15) to eliminate $M$ and write the ground state energy as a function of $\delta$ only. We then obtain the final expression of the ground state energy as:

$$E_0(\delta, h) = -\frac{J}{\pi} \left[ \sqrt{(1 - \delta)^2 - \left(\frac{h}{J}\right)^2} + \frac{h}{J} \arcsin \left(\frac{h}{J(1 - \delta)}\right) \right] + K \delta^2 + \frac{h}{2}$$  \hspace{1cm} (16)

if $|h| < J|1 - \delta|$ and:

$$E_0(\delta, h) = \frac{K}{2} \delta^2 - \frac{h}{2}$$  \hspace{1cm} (17)

if $|h| > J|1 - \delta|$. The Eq. (16) describes the XX chain not fully polarized, whereas Eq. (17) describes the fully polarized XX chain. The function $E_0(\delta, h)$ is plotted as a function of $\delta$ for different values of $h/J$ on Fig. 11. As is evident on Fig. 11, as $h$ is increased above $h_c$, the minimum existing for $\delta = \delta_c < 0$ acquires a higher energy than the minimum at $\delta = 0$ (see Figs. 11(b)-(c)-(d)). As a result, at $h = h_c$, the parameter $\delta$ jumps from $\delta_c$ to 0. Eq. (16) then implies that the magnetization also jumps from a value $M = M_c$ to $M = 1/2$. In other words, the system presents a first order transition at $T = 0$ as a function of the magnetic field. In physical terms, the origin of this first order transition is easy to grasp. When the system described by (11) is in the spin gap state, it does not contain any triplet. When the system starts to be polarized, the triplets first occupy the states with the most negative kinetic energy. Due to the hard-core repulsion, instead of being all in the lowest energy state, they form a Fermi-sea. By contracting, the lattice increases the exchange energy and thus makes the kinetic energy of this Fermi sea more negative. In turn, this favors the condensation of a larger number of triplets in the Fermi-sea, and a further decrease of the energy of the triplets. This process is only limited by the loss of elastic energy coming from the deformation of the lattice. The natural consequence is that as soon as the magnetic field overcomes the gap, a finite density of triplets appear. Due to the fact that the triplets form a Fermi sea, their Bose condensation is incomplete and this limits the density of triplets. In the magnetized state, the system of coupled ladders possesses a quasi-long range magnetic order with:

$$\langle S_{n,m}^+ S_{n',m}^- \rangle \sim \frac{(-)^{n-n'} + \cos[\pi(1 - 2\tilde{m})]}{|n-n'|^{1/2}},$$  \hspace{1cm} (18)

$$\langle S_{n,m}^z S_{n',m}^z \rangle \sim \frac{\tilde{m}^2}{4} + \frac{1}{|n-n'|^2} + \frac{\cos[2\pi \tilde{m}]}{|n-n'|^2},$$  \hspace{1cm} (19)

$\tilde{m} = M + 1/2$ being the magnetization per rung of the ladder. The power-law decay of the correlations of the staggered transverse magnetization can be interpreted as a quasi Bose condensation of the hardcore bosons of the ladder in the lowest energy state of momentum $(\pi, \pi)$. In fact, even in a quasi-one dimensional array of coupled chain, a long range order of the BEC order parameter can develop. The reason is that in any real system, besides the spin-phonon coupling, there exists also an interladder exchange coupling $J' S_{n,2m-1}^z S_{2,2m+1}^z$. If this interladder coupling is small enough compared to the rung coupling $J_2$, the singlet phase is stable, and no antiferromagnetic ordering is observed in the absence of an applied magnetic field. In the magnetized state however, this interladder coupling gives rise at $T = 0$ to a long range ordering of the spins. In our problem, the Luttinger exponent being equal to one, it is easily seen using the results of Ref. 13 that the staggered magnetization in the plane perpendicular to applied field behaves as $(J'/J_2)^{1/6}$. Therefore, one should also expect a discontinuity of the staggered magnetization from 0 to $(J'/J)^{1/6}$ as the coupled ladder system becomes magnetized. This discontinuity is the signature of the BEC long range order of the triplet bosons in the magnetized state.
FIG. 1: The ground state energy as a function of $\delta$ for different values of the magnetic field $h$. (a) For low field, there is a single minimum at $\delta < 0$. (b) For a higher field $h > h_{c<}$, a second minimum, at a higher value of the energy is present. This second minimum corresponds to a metastable state. (c) For a critical value of the magnetic field, the two minimum become degenerate. (d) Above the critical field, the absolute minimum of the ground state energy is for $\delta = 0$. A metastable minimum exists for $\delta < 0$. (e) For $h = h_{c>}$, the minimum at $\delta < 0$ becomes unstable. (f) Above $h_{c>}$, the only minimum is for $\delta = 0$. In the range of $h_{c<} < \delta < h_{c>}$, hysteresis in $\delta$ as $h$ is varied is expected.

2. Analytic study of the minimum of the enthalpy

We now turn to an analytic study of the dependence of the parameter $\delta$ on the magnetic field. In terms of $\delta$, the condition \[(c)\] for the existence of the minimum can be rewritten as:

$$K \delta + p = -\frac{1}{\pi} \sqrt{J^2 - \frac{h^2}{(1 - \delta)^2}}$$  \hspace{1cm} (20)

This equation is rewritten as the following equation of the fourth degree:

$$\delta^4 + 2 \left( \frac{p}{K} - 1 \right) \delta^3 + \left[ 1 - 4 \frac{p}{K} + \left( \frac{p}{K} \right)^2 - \left( \frac{J}{\pi K} \right)^2 \right] \delta^2 + 2 \left[ \left( \frac{J}{\pi K} \right)^2 + \frac{p}{K} - \left( \frac{p}{K} \right)^2 \right] \delta + \frac{h^2 - J^2}{(\pi K)^2} + \left( \frac{p}{K} \right)^2 = 0.$$  \hspace{1cm} (21)

It can be solved by the method of Cardan as exposed in Ref. \[59\] p. 17, sec. 3.8.3. The dependence of $\delta$ on $h$ is represented on figure \[p\] and the resulting magnetization on figure \[3\].
It can be shown that the lattice parameter given by the solution of (21) has a discontinuity as a function of the magnetic field for a critical field $h_{c_>} \geq h_c$ given by:

$$\left( \frac{h_{c_>}}{J} \right)^2 = \frac{7}{8} + \frac{7p}{4K} + \frac{5}{8} \left( \frac{p}{K} \right)^2 + \left( \frac{p}{K} \right)^3 + \frac{1}{4} \left( \frac{J}{\pi K} \right)^2 + \frac{1}{4} \left( \frac{1 + \frac{p}{K}}{\sqrt{1 + \frac{p}{K}}} \right)^2 + \frac{8p}{\pi} + 2 \left( \frac{p}{K} \right)^2. \hspace{1cm} (22)$$

For a field just below $h_{c_>}$, the value of $\delta$ is given by:

$$\delta_{c_>} = -\frac{p}{K} + \frac{1}{4} \left[ 1 + \frac{p}{K} - \sqrt{\left( 1 + \frac{p}{K} \right)^2 + 8 \left( \frac{J}{\pi K} \right)^2} \right]. \hspace{1cm} (23)$$

and above $h_{c_>$, the value of $\delta$ is simply $\delta = 0$ as there are no physical solutions to the equation (21). The behavior of the enthalpy as a function of $\delta$ for $h = h_{c_>$ is represented on Fig. 1(e).

For $\delta = \delta_{c_>$, the corresponding magnetization is $M_{c_>$ such that:

$$\cos(\pi M_{c_>} J) = \frac{J}{\pi(K + p) + \pi \sqrt{(K + p)^2 + 8J^2}}. \hspace{1cm} (24)$$

As with all first order transition, the solution of Eq. (21) may only describe a metastable state and not the true minimum of the enthalpy, and the true thermodynamic transition happens for a field $h_c$ lower than $h_{c_>}$. This is clearly seen on Fig. 1. As a result, the field $h_{c_>$ only corresponds to an extremity of the hysteresis cycle of the magnetization loop. The other extremity of the hysteresis cycle is obtained when the minimum at $\delta = 0$ becomes unstable, i.e. when the second derivative of the enthalpy w.r.t. $\delta$ becomes negative for $\delta = 0$. The corresponding critical field is given by $h_{c_<} = J(1 + p/K)$. Obtaining analytically the true thermodynamic critical field is difficult in the general case. However, in the case of a stiff lattice this can be done easily using a Landau-Ginzburg expansion.

FIG. 2: Striction for $T = 0, P = 0, K = 1, J = 1$. This is obtained from the solution of Eq. (21). It does not correspond to the thermodynamic striction which presents a jump for $h = h_c < h_{c_>}$.
FIG. 3: magnetization for \( T = 0, P = 0, K = 1, J = 1 \). This is obtained from the solution of Eq. (21) and this is not the thermodynamic magnetization.

3. Landau-Ginzburg expansion at \( T = 0 \)

A more detailed description of the first order transition can be obtained in the limit of very small magnetization jump, when it is possible to expand the ground state energy in powers of \( M - 1/2 \). Expressing the ground state energy as a function of \( M \) only, using the Eqs. (13) and (14), we find:

\[
E(M) = -\frac{J^2}{2\pi^2 K} \cos^2(\pi M) - \frac{J}{\pi} \left(1 + \frac{p}{K}\right) \cos(\pi M) - hM - \frac{p^2}{2K} \tag{25}
\]

It is convenient to subtract the energy of the fully polarized system \( E(M = 1/2) = -h/2 - p^2/(2K) \) to \( E(M) \) and work with the quantity:

\[
E_0(M) = -\frac{J^2}{2\pi^2 K} \cos^2(\pi M) - \frac{J}{\pi} \left(1 + \frac{p}{K}\right) \cos(\pi M) - h \left(M - \frac{1}{2}\right) \tag{26}
\]

Expanding Eq. (26) to third order in \( M - 1/2 \), we obtain:

\[
E_0(M) = -\frac{\pi^2 J}{6} \left(1 + \frac{p}{K}\right) \left(M - \frac{1}{2}\right)^3 - \frac{J^2}{2K} \left(M - \frac{1}{2}\right)^2 + \left[J \left(1 + \frac{p}{K}\right) - h\right] \left(M - \frac{1}{2}\right) \tag{27}
\]

It is important to note that since \( M < 1/2 \), the negative coefficient of the cubic term does not lead to any instability. Minimizing the ground state energy with respect to \( M \), one finds:

\[
\left[J \left(1 + \frac{p}{K}\right) - h\right] - \frac{J^2}{K} \left(M - \frac{1}{2}\right) + \frac{\pi^2 J}{2} \left(1 + \frac{p}{K}\right) \left(M - \frac{1}{2}\right)^2 = 0 \tag{28}
\]

For \( h/J > (1 + p/K) + J^2/[2\pi^2 K(K + p)] \approx h_{c3} \), this equation has no solution. In this regime, \( E_0(M) \) is a uniformly decreasing function of \( M \) and the minimum is obtained for \( M = 1/2 \) corresponding to the fully saturated case. For \( h/J < (1 + p/K) + J^2/[2\pi^2 K(K + p)] \), the equation (28) admits two solutions:

\[
M_{</>} = \frac{1}{2} - \frac{J}{K} \pm \frac{\sqrt{\left(\frac{J}{K}\right)^2 - \frac{2\pi^2}{2} \left[1 + \frac{p}{K} - \frac{h}{J}\right] \left(1 + p/K\right)}}{\pi^2 \left(1 + \frac{p}{K}\right)} \tag{29}
\]
When \( h/J < 1 + p/K = h_{c_+} \), the solution \( M > \) becomes larger than \( 1/2 \) and thus unphysical. In this regime, \( M_- \) is an absolute minimum of \( E_0(M) \). Let us first consider the intermediate regime \( h_{c_+} < h/J < h_{c_-} \). In this regime, there is a minimum of \( E_0(M) \) for \( M = M_- \), a maximum for \( M = M_+ \), and a second minimum for \( M = 1/2 \). The exchange of stability of these two minima is at the origin of the first order transition. We have \( E_0(1/2) = 0 \), therefore, the stability of the minimum at \( M = M_- \) depends only on the sign of \( E_0(M_-) \). Using the equation (28), we can rewrite:

\[
E_0(M_-) = \left( M_- - \frac{1}{2} \right)^2 \left[ \frac{J}{2K} + \frac{\pi^3}{3} \left( 1 + \frac{p}{K} \right) \left( M_- - \frac{1}{2} \right) \right].
\]  

(30)

The stability of the two minima at \( M = 1/2 \) and \( M = M_- \) is thus exchanged when:

\[
\frac{J}{2K} = -\frac{\pi^2}{3} \left( 1 + \frac{p}{K} \right) \left( M_- - \frac{1}{2} \right).
\]  

(31)

At that point, one has:

\[
M_- = \frac{1}{2} - \frac{3J}{2\pi^2(K + p)}
\]  

(32)

and the magnetization jump at the transition is:

\[
\Delta M = \frac{3J}{2\pi^2(K + p)}.
\]  

(33)

From this expression we immediately see that the condition of applicability of the Landau-Ginzburg expansion is \( J \ll (K + p) \), that is equivalent to consider a very stiff lattice or a very high pressure. Using the equation (14), it is also possible to obtain an expression of the lattice parameter as:

\[
\delta = -\frac{p}{K} + \frac{J}{K} \left( M - \frac{1}{2} \right) = -\frac{p}{K} - \frac{3J^2}{2\pi^2(K + p)}
\]  

(34)

At the transition the jump of the lattice parameter is thus:

\[
\Delta \delta = \frac{J}{K} \delta M = \frac{3J^2}{2\pi^2(K + p)}.
\]  

(35)

The magnetic field at the transition is given by Eq. (15) as:

\[
\frac{h_c}{J} = 1 + \frac{p}{K} + \frac{3J^2}{8\pi^2K(K + p)}.
\]  

(36)

and obviously we have \( h_{c_+} < h_c < h_{c_-} \). As we have already mentioned, in the intermediate regime, hysteresis can be observed as there are two minimas, one of them being metastable. This is shown on Fig. 4 where the energy for \( dE/dM = 0 \) becomes superior to the energy of the fully saturated state at \( h > h_c \). At that point the thermodynamic minimum becomes \( M = 1/2 \), and the branch with \( dE/dM = 0 \) becomes metastable. When the field is increased sufficiently rapidly, the magnetization may remain on the metastable branch until the field reaches \( h_{c_+} \). When the field is decreased from \( h_{c_+} \), at \( h_c \) the solution with \( M = 1/2 \) becomes metastable, and for a sufficiently rapid decrease of the magnetic field, one can have a magnetization \( M = 1/2 \) until the magnetic field reaches \( h_{c_-} \). This is the origin of the hysteresis cycle in the magnetization. In Fig. 4 is shown a plot of the hysteresis cycle of the magnetization for \( T = 0 \). A similar hysteresis cycle exists for the distortion and is observed in Fig. 3 of Ref. 35, albeit in the vicinity of \( H = H_{c_+} \). In agreement with our picture, when the field is decreased, the system remains on the metastable distorted state, and when the distorted state becomes unstable the lattice parameter jumps to its value in the undistorted state. When the field is increased, the system remains in the metastable undistorted state until it becomes unstable.

Returning to our model, we note that the application of pressure is pushing the first order transition to higher value of the applied magnetic field. This can be understood as a consequence of the fact that in the distorted state \( \delta < 0 \) and \( |\delta| \) is higher than in the undistorted state. As a result, the stability of the distorted state is increased by the application of pressure. Also, the hysteresis cycle becomes narrower as pressure is increased. An analogous effect is observed in ferromagnets\(^{13}\), where application of pressure reestablishes the second order Curie transition. It might be interesting to investigate the effect of pressure on the transition studied in Ref. 35 to see if the behavior of \( H_{c_+} \) as a function of pressure is in agreement with our prediction.
FIG. 4: Hysteresis cycle for $T = 0$ and $K = J = 1, P = 0$. The thermodynamic transition happens for $h = h_c \simeq 1.03J$, however the distorted state is metastable for $h_c < h < h_{c>} \simeq 1.045J$ and the undistorted state is metastable in the region $h_{c<} = J < h < h_c$. As the field $h$ is increased from 0 to $h_{c>}$, the system remains on the metastable branch, and the magnetization jumps to $1/2$ at $h = h_{c>}$. As the magnetic field is decreased, the magnetization drops from $1/2$ at $h = h_{c<}$. This produces an hysteresis cycle in the magnetization. A similar hysteresis cycle is expected for the lattice distortion.

B. Behavior of susceptibilities in the distorted phase

Now that we have described the first order transition, we would like to discuss the effect of the spin-phonon coupling on the susceptibilities of the system in the distorted phase. The following susceptibilities are of interest to us:

the compressibility:

$$\tilde{\kappa} = -\left(\frac{\partial \delta}{\partial p}\right)_h,$$

(37)

the magnetic susceptibility:

$$\chi = -\left(\frac{\partial M}{\partial h}\right)_p,$$

(38)

and the parameter:

$$\Lambda = -\left(\frac{\partial \delta}{\partial h}\right)_p = \left(\frac{\partial M}{\partial p}\right)_h,$$

(39)

measuring the Joule effect and its reciprocal, the Villari effect. The two equivalent definitions of $\Lambda$ are direct consequences of the definitions $M = -\left(\frac{\partial G}{\partial h}\right)_p$, $\delta = \left(\frac{\partial G}{\partial p}\right)_h$. The equation of state results from the Eqs. (14-15).

Differentiating the second equation w.r.t. $p$, we find:

$$\left(\frac{\partial M}{\partial p}\right)_h = \frac{\tan(\pi M)}{\pi(1 - \delta)} \left(\frac{\partial \delta}{\partial p}\right)_h$$

(40)

This equation indicates that applying a pressure for fixed magnetic field induces a change of magnetization (Villari effect), related to the compressibility. Differentiating the first equation w.r.t. $p$, instead gives:

$$K \left(\frac{\partial \delta}{\partial p}\right)_h + 1 - J \sin(\pi M) \left(\frac{\partial M}{\partial p}\right)_h = 0$$

(41)
Using Eq. (40), we finally obtain the following expression for the compressibility:

\[
\frac{1}{\kappa} = - \left( \frac{\partial \delta}{\partial p} \right)_h = \frac{1}{K - \frac{J}{\pi(1 - \delta)} \tan(\pi M) \sin(\pi M)}
\]  

We see that the compressibility of the system (which is in one dimension the inverse of the elastic constant) is enhanced by the interaction with the spin excitations. The physical reason is that when the lattice spacing is diminished, the magnetic energy is increased, which compensates for the loss of elastic energy. Expressed in terms of \( \delta \), using Eq. (15), the elastic constant reads:

\[
\kappa = K - \frac{1}{\pi (1 - \delta)^2} \sqrt{J^2(1 - \delta)^2 - h^2}
\]

The behavior of \( \kappa \) is represented on Fig. 5. It presents a minimum for \( h = h_c \). The jump of the elastic constant from a low value to its original value as the magnetic field is increased, implies a minimum in elastic constant as a function of magnetic field. At zero temperature such minimum appears more like a dip. Experimentally, the presence of such a dip near the saturation field is known as “\( \Delta E \)” effect in ferromagnetic materials. Using Eqs. (36) and (34), we obtain that the minimum value of the elastic constant reads for \( J \ll K \):

\[
\kappa_c = K \left[ \frac{1}{3} + \frac{29}{16} \left( \frac{J}{\pi(K + p)} \right)^2 \right],
\]

showing that the elastic constant can be reduced to \( 1/3 \) of its value in the fully polarized phase. Applying pressure tends to diminish further the value of \( \kappa_c \). The behavior of \( \kappa \) as a function of an applied magnetic field has been recently measured in a spin 1/2 Heisenberg chain material, the coordination polymer CuCCP, via sound velocity measurements. These experiments reveal a pronounced minimum at the saturation field in qualitative agreement with the behavior represented on fig. 5. We will not attempt a quantitative comparison because the proper model to use to study the anomaly in the elastic constant of CuCCP is the Heisenberg model coupled to acoustic phonons and the thermodynamics of this model, even in the mean field approximation requires a much more sophisticated approach than the one of the present paper.

![FIG. 5: The effective elastic constant as a function of the magnetic field. Below the saturation field, \( h = h_c \), the elastic constant is very sharply reduced. For \( h = h_c \), the effective elastic constant jumps to \( K \). The curve is drawn for \( J = K = 1 \).](image-url)
The most characteristic signature of magnetostriction is the change of magnetization under applied pressure. It is measured by:

\[ \Lambda = \left( \frac{\partial M}{\partial p} \right)_h = -\frac{\tan(\pi M)}{\pi K(1 - \delta) - J \tan(\pi M) \sin(\pi M)} = -\left( \frac{\partial \delta}{\partial h} \right)_p, \]

(45)

The behavior of \( \Lambda \) is reported on Fig. 4. The application of pressure leads to a diminution of the magnetization, and the application of a magnetic field in an increase of the lattice parameter, which indicates that the system has a positive magnetostriction\(^{40}\). The variation of the magnetization \( \Lambda \) is an interesting quantity to measure, as well as \( \left( \frac{\partial \delta}{\partial h} \right) \), because they are non-zero only in the phase that is not fully polarized, and their equality is the very signature of magnetostriction.

By considering the derivative of the equations of state (14-15) w.r.t. \( h \), we derive the magnetic susceptibility. Differentiating the first equation gives:

\[ \left( \frac{\partial \delta}{\partial h} \right)_p = \frac{J}{K} \sin(\pi M) \left( \frac{\partial M}{\partial h} \right)_p \]

(46)

Differentiating the second equation (15) then yields for the susceptibility:

\[ \chi = \left( \frac{\partial M}{\partial h} \right)_p = \frac{1}{\pi J \left[ (1 - \delta) \cos(\pi M) - \frac{J}{\pi K} \sin^2(\pi M) \right]} \]

(47)

The magnetic susceptibility can be rewritten as:

\[ \chi = \chi_0(h, J(1 - \delta)) \frac{K}{\kappa}, \]

(48)

where \( \chi_0(h, J) \) is the magnetic susceptibility of an XX spin 1/2 chain with exchange constant \( J \) in a magnetic field \( h \). We thus see that the susceptibility is strongly enhanced with respect to the case of a perfectly rigid lattice. A plot of \( \chi \) is reported in Fig. 4. The susceptibility has a maximum for \( h = h_c \), and then falls to zero. Using Eqs. (34) and (36), we find that the maximum susceptibility is:

\[ \chi_c = \frac{K}{J^2} \frac{3}{1 + \frac{189}{32} \left( \frac{J}{\pi (K + p)} \right)^2}, \]

(49)

and thus the maximum value of the susceptibility is proportional to the elastic modulus in the fully polarized phase. We also note that applying pressure results in an increase of the maximal susceptibility. With the expressions of \( \Lambda \) (Eq. 40) and \( \chi \) (47), we see that we have the following relation:

\[ (1 - \delta) \frac{\Lambda}{\chi} = \frac{h}{K}. \]

(50)

### IV. POSITIVE TEMPERATURE

At fixed magnetic field and fixed pressure, we can vary the temperature and the numerical analysis of the free energy as a function of temperature shows that above a certain temperature, the metastable minimum disappears, and one is left with a single minimum. This behavior is illustrated for \( P = 0 \) and \( K = J = J \) on Fig. 8. As a result, above a certain temperature, the first order transition as a function of the magnetic field disappears and is replaced by a crossover. This is the analog of the critical point in the Van der Waals mean field theory of the liquid-gas transition. In the present problem, the role of the pressure is played by the magnetic field. Applying the magnetic field is analogous to applying a pressure to the Van der Waals fluid to liquefy it. It is important to point out that the temperature at which the second minimum as a function of \( \delta \) disappears is a function of the applied magnetic field. The second minimum disappears at lower temperature when its energy is noticeably higher that the energy of the stable minimum. As a result, the width of the hysteresis cycle decreases as a function of temperature. A second effect of temperature is to blur the distinction between the fully magnetized phase and the partially magnetized phase. This effect can be seen on Fig. 8. As temperature is increased, the stable minimum which corresponds to \( \delta = 0 \) is moved to \( \delta < 0 \). Thus, as the magnetic field is decreased for \( T > 0 \), a reduction of the magnetization is observed even before the magnetization jumps, in contrast with the behavior for \( T = 0 \).
FIG. 6: The magnetic susceptibility as a function of the magnetic field. It diverges at the critical field where the transition takes place. The plot is done for $J = K = 1$.

FIG. 7: The Joule coefficient $\Lambda = \left( \frac{\partial M}{\partial p} \right)_h = - \left( \frac{\partial M}{\partial h} \right)_p$ as a function of the magnetic field. We see that applying pressure results in a decrease of the magnetization which indicates a positive magnetostriction. The plot is done for $J = K = 1$. 
FIG. 8: The evolution of the free energy as a function of temperature for $K = J = 1$ and $h = 1.04$. At zero temperature, the double minima are neatly visible. The absolute minimum corresponds to $\delta = 0$ indicating a non-magnetized phase, without deformation. For not too large positive temperature, the two minimum are still visible, but the barrier between them becomes smaller. Also, one notices that the minimum of the free energy corresponds to a solution with $\delta < 0$, indicating a contraction of the lattice as $T$ increases, i.e. a negative dilatation coefficient. As temperature is further increased, i.e. for $T = 0.03J$, there is only a single minimum indicating the disappearance of the first order transition.

A. Ginzburg-Landau expansion at finite $T$

In this section, we turn to the derivation of the Ginzburg-Landau expansion at finite temperature. Such expansion is derived from the free energy:

$$F(T, \delta, h) = K \frac{\delta^2}{2} - \frac{1}{\beta} \int \frac{dk}{2\pi} \ln(1 + e^{-\beta[(1-\delta)\epsilon(k) - h]}),$$

in the vicinity of $\delta = 0$. Performing the Taylor expansion in the logarithmic function, we find:

$$F(T, \delta, h) = -\delta \int \frac{dk}{2\pi} \frac{\epsilon(k)}{e^{\beta(\epsilon(k) - h)}} + \left( K - \beta \int \frac{dk}{8\pi} \frac{\epsilon(k)^2}{\cosh^2 \left( \frac{\beta}{2} (\epsilon(k) - h) \right)} \right) \frac{\delta^2}{2}$$

$$- \beta^2 \int \frac{dk}{2\pi} \frac{\epsilon^3(k)}{\cosh^3 \left( \frac{\beta}{2} (\epsilon(k) - h) \right)} \frac{\delta^3}{24} + \beta^2 \int \frac{dk}{2\pi} \frac{\epsilon^4(k)}{\cosh^4 \left( \frac{\beta}{2} (\epsilon(k) - h) \right)} \frac{\delta^4}{192}.$$  

The solution with $\delta = 0$ becomes unstable when:

$$K(T) = K - \beta \int_{-\pi}^{\pi} \frac{dk}{8\pi} \frac{\epsilon(k)^2}{\cosh^2 \left( \frac{\beta}{2} (\epsilon(k) - h) \right)} < 0.$$  

At low temperature, we can estimate $K(T)$ as:

$$K(T) = K - \frac{1}{\pi} \left\{ \frac{h^2}{\sqrt{J^2 - h^2}} + \frac{\pi^2 T^2}{6} \frac{1}{\sqrt{J^2 - h^2}} \left[ 2 + \frac{h^2 (J^2 + 2h^2)}{(J^2 - h^2)^2} \right] \right\}.$$  

(51)
Thus, the thermal correction can be neglected if:

$$\frac{\pi^2}{6} T^2 \left[ \frac{2}{h^2} + \frac{J^2 + 2h^2}{(J^2 - h^2)^2} \right] \ll 1,$$

(55)

This leads for $J \simeq h$ to:

$$T \ll \frac{8}{\pi^2} |J - h|$$

(56)

Except for a small region of size of order $\pi^2/8T$ around $J$, the thermal correction to the stability of the undistorted solution is negligible for low temperatures. This leads us to expect that the first order transition persists for non-zero but sufficiently low temperatures. We now show that there is a temperature $T_\ast$ above which the first-order transition as a function of the magnetic field disappears. Using a straightforward minoration $\cosh(x) \geq 1$ term in Eq. (53), we find that:

$$K - \frac{J^2}{8T} < K(T),$$

(57)

and when:

$$K > \frac{J^2}{8T},$$

(58)

i.e. $T > J^2/(8K)$, we have $K(T) > 0$ and thus above a temperature $T_\ast = J^2/(8K)$, there is certainly no first order transition. As an aside, we note that the bound (58) can be improved when $h > J$. Then, $\cosh[(\epsilon(k) - h)/(2T)] < \cosh[(J - h)/(2T)]$ and

$$K - \frac{J^2}{8T \cosh^2 \left( \frac{J - h}{2T} \right)} < K(T),$$

(59)

which shows that for low temperature, the solution with $\delta = 0$ remains stable for high fields. We now proceed to show that for $h < J$ an upper bound for $K(T)$ can also be found in the regime of $|h| < J$. Using this bound, we can show that the solution with $\delta = 0$ is unstable at low but finite temperature on a soft lattice. This shows that the first order transition can be observed for $T > 0$ in that case. To obtain the bound, we use $k_F$ defined by $\epsilon(k_F) = h$ and write:

$$\epsilon(k) - h = -J(\cos k - \cos k_F) = 2J \sin \left( \frac{k - k_F}{2} \right) \sin \left( \frac{k + k_F}{2} \right)$$

(60)

We have for $k > 0$ the obvious majoration:

$$|\epsilon(k) - h| < J|k - k_F|$$

(61)

Therefore:

$$\cosh^2 \frac{\epsilon(k) - h}{2T} < \cosh^2 \frac{J|k - k_F|}{2T},$$

(62)

and:

$$K(T) < K - \int_0^{\pi} \frac{dk}{\pi T} \frac{J^2 \cos^2 \frac{k}{2T}}{4 \cosh^2 \frac{J(k - k_F)}{2T}}$$

(63)

By a change of variables, this is rewritten as:

$$K(T) < K - \frac{2J}{\pi} \int_{\pi-k_F}^{\pi} \frac{dx}{\sqrt{T \pi T}} \frac{4 \cos^2 \left( k_F + \frac{2T x}{J} \right)}{\cosh^2 x}$$

(64)

In the limit $Jk_F \gg T$ and $J(\pi - k_F) \gg T$, it is possible to calculate approximately the upper bound as:

$$K - \frac{J}{2\pi} \left[ 1 - \frac{2\pi T}{\sinh \frac{2\pi T}{J}} \cos 2k_F \right] + O(e^{-J/T \min(k_F, \pi-k_F)}),$$

(65)
which shows that when \( K < J/(2\pi) \), the instability exists for low temperature \( T \ll J \text{Min}(k_F, \pi - k_F) \). The first order phase transition can therefore be observed at positive temperature at least when the lattice is sufficiently soft.

We now turn to an estimation of the temperature at which the first order transition disappears valid in the case of a stiff lattice. First, we express \( K(T) \) using the density of states. We have:

\[
K(T) = K - \int_{-J}^{J} \frac{d\epsilon}{\pi \sqrt{J^2 - \epsilon^2}} \frac{\epsilon^2}{4 \cosh^2 \left( \frac{\epsilon - h}{2T} \right)}
\]

(66)

The divergence of the density of state for \( \epsilon \to J \) is responsible for the instability. Therefore, it is legitimate, when \( |J - h| \ll J \) to expand the integrand in Eq. (66) for \( \epsilon \to J \). We find:

\[
K(T) = K - \int_{-J}^{J} \frac{d\epsilon}{\pi \sqrt{2J(J - \epsilon)}} \frac{J^2}{4 \cosh^2 \left( \frac{\epsilon - h}{2T} \right)}
\]

(67)

Performing the change of variable \( \epsilon = J - (J - h)x \), we can rewrite the integral in Eq. (67) as:

\[
K(T) = K - \frac{J^{3/2}}{\pi \sqrt{2(J - h)}} \mathcal{F} \left( \frac{J - h}{T} \right),
\]

(68)

where:

\[
\mathcal{F}(y) = \int_{0}^{\infty} \frac{dx}{\sqrt{\pi}} \frac{y}{4 \cosh^2 \left[ \frac{y}{2}(1 - x) \right]}
\]

(69)

It is easy to see that \( \mathcal{F}(y \to \infty) = 1 \) and \( \mathcal{F}(y \to 0) \sim y^{1/2} \). As a result, at low temperature, \( T \ll (J - h) \), we recover the zero temperature result, and at high temperature \( J \gg T \gg (J - h) \), we find that:

\[
K(T) = K - \frac{J^{3/2}}{2\pi T^{1/2}},
\]

(70)

and if \( T > T_c \) where:

\[
\frac{T_c}{J} = \frac{J^2}{(2\pi K)^2}
\]

(71)

the solution \( \delta = 0 \) becomes stable, indicating that the first order transition disappears. We note that given the exponential temperature dependence of the spin-Peierls transition temperature \( 38 \), the first order transition appears at a much higher temperature than the spin-Peierls transition in the case of a stiff lattice.

B. Numerics

By the minimization of the Gibbs free energy \( 10 \) w.r.t. \( \delta \), we have obtained the \( T \) dependence of the striction and the magnetization.

We find that the discontinuity in \( \delta \) or \( M \) becomes smaller as \( T \) is increased. Also, we note there is a finite striction and a magnetization slightly below 1/2 in the high \( h \) phase. The reason for this is that at finite temperature, pseudofermion excitations are created which results in a lowering of the absolute value of the kinetic energy-like term in Eq. \( 11 \). As a result, the absolute value of \( \delta \) is diminished in the partially magnetized phase and increased in the polarized phase. Above a certain temperature, the discontinuity is replaced by a large slope, indicating a continuous crossover from the fully polarized to the unpolarized state. This behavior is reminiscent of the liquid-gas transition in the Van der Waals fluid \( 58 \). For \( J = K = 1 \), we find the transition temperature to be of order 0.03\( J \) in reasonable agreement with Eq. \( 71 \).

C. Susceptibilities at positive temperature

For positive temperatures, the equation of state is obtained from the equations:

\[
K \delta + p = \int \frac{dk}{2\pi} \frac{\epsilon(k)}{1 + e^\beta(1-\delta)\epsilon(k)-h}
\]

(72)

\[
M = \int \frac{dk}{2\pi} \left[ \frac{1}{1 + e^\beta(1-\delta)\epsilon(k)-h} - \frac{1}{2} \right]
\]

(73)
FIG. 9: The striction as a function of the magnetic field for various temperatures and $K = J = 1$. For $T = 0.01$, the discontinuity becomes smaller than for $T = 0$ but it is still present. For $T = 0.03$ the discontinuity disappears, and is replaced by a rapid but continuous change of $\delta$. For $T = 0.1$, the change becomes even more gradual. One can notice that $\delta$ reaches zero at higher field when the temperature is increased.

FIG. 10: The magnetization as a function of the magnetic field for various temperatures and $K = J = 1$. For $T = 0.01$, the discontinuity is smaller, but it is still present. For $T = 0.03$ discontinuity disappears, and is replaced by a rapid but continuous change of $M$. As temperature is further increased, the change of $M$ becomes more gradual. One can notice that as $T$ is increased, the saturation field becomes higher.
Taking the derivative of the first equation w.r.t. \( h \) yields:

\[
\left( \frac{\partial \delta}{\partial h} \right)_{T,p} = \frac{\beta \int \frac{dk}{2\pi} \frac{e(k)}{4 \cosh^2 \frac{\beta}{2}[(1-\delta)e(k)-h]}}{K - \beta \int \frac{dk}{2\pi} \frac{e(k)}{4 \cosh^2 \frac{\beta}{2}[(1-\delta)e(k)-h]}} = -\Lambda
\] (74)

The behavior of the Joule coefficient as a function of the magnetic field at finite temperature is reported in Fig. 11. At very low temperatures it presents a cusp like behavior with a jump at the critical field \( h_c \). As the temperature increases the cusp is replaced by a maximum for \( h = h_M(T) < h_c \) that becomes broader at increasing \( T \).

\[
\begin{aligned}
\text{FIG. 11: Derivative of the lattice parameter w.r.t. } &h \text{ and varying the temperature. The plot is done for } J = K = 1. \text{ Below the transition temperature, the discontinuity is visible. Above the transition temperature, the discontinuity is replaced by a maximum. As the temperature increases, this maximum is lowered, and the region of anomaly is broadened.}
\end{aligned}
\]

Taking the derivative of the second equation w.r.t. \( h \) then gives:

\[
\left( \frac{\partial M}{\partial h} \right)_{T,p} = \beta \int \frac{dk}{2\pi} \frac{1}{4 \cosh^2 \frac{\beta}{2}[(1-\delta)e(k)-h]} + \frac{\left( \beta \int \frac{dk}{2\pi} \frac{e(k)}{4 \cosh^2 \frac{\beta}{2}[(1-\delta)e(k)-h]} \right)^2}{K - \beta \int \frac{dk}{2\pi} \frac{e(k)}{4 \cosh^2 \frac{\beta}{2}[(1-\delta)e(k)-h]}}
\] (75)

The plot of the magnetic susceptibility at finite temperature is reported in Fig. 12. The singularity below \( T_c \) is changed into a maximum above \( T_c \).

Similarly, taking the derivative of the first equation w.r.t. \( p \) yields:

\[
\frac{-1}{\kappa} = \left( \frac{\partial \delta}{\partial p} \right)_{T,h} = \frac{-1}{K - \beta \int \frac{dk}{2\pi} \frac{e(k)^2}{4 \cosh^2 \frac{\beta}{2}[(1-\delta)e(k)-h]}}
\] (76)

At finite temperature the effective elastic constant is thus given by:

\[
\kappa_T = K - \beta \int \frac{dk}{2\pi} \frac{e(k)^2}{4 \cosh^2 \frac{\beta}{2}[(1-\delta)e(k)-h]}
\] (77)

As shown in Fig. 13 the dip in the elastic constant at \( T = 0 \) (cf. Fig. 5) as a function if the magnetic field is replaced by a minimum as the temperature \( T > T_c \). The the \( T \) dependence of the elastic constant is very reminiscent of
the results reported in Ref. [44] with the dip becoming broader and less pronounced as the temperature is increased. However, in this reference, the behavior of the elastic constant was only discussed in a phenomenological way, by introducing an interaction proportional to the striction and the square of the magnetization, i.e., a term $-\delta\langle S^z \rangle^2$. A more quantitative approach could be developed by treating the Hamiltonian \( H \) by a TBA mean-field theory.

Finally, taking the derivative of the second equation with respect to \( p \) allows one to check that Eq. (74) is recovered.

### D. Other thermodynamic quantities: Dilatation coefficient and specific heat

Besides the susceptibilities considered in the zero temperature case, and recalculated at positive \( T \), there are some other quantities that can be defined for finite temperature, namely the dilatation coefficient:

\[
\alpha = -\left( \frac{\partial \delta}{\partial T} \right)_{p,h}, \tag{78}
\]

the specific heat:

\[
C_p = -\left( \frac{\partial H}{\partial T} \right)_{p,h}, \tag{79}
\]

where \( H \) is the enthalpy, and the quantity:

1. Specific heat

The internal energy is given by:

\[
U(T, \delta, h) = \frac{\partial}{\partial \beta} \left( \frac{F(T, \delta, h)}{T} \right) = \frac{K\delta^2}{2} + \int \frac{dk}{2\pi} \frac{[(1-\delta)\epsilon(k) - h]}{1 + e^\beta[(1-\delta)\epsilon(k)-h]}, \tag{80}
\]
The effective elastic constant as a function of the magnetic field and different temperatures. The curve is drawn for $J = K = 1$. We notice that in the fully polarized state at low temperature, the elastic constant quickly returns to its value in the absence of interaction with magnetic excitations. A jump of elastic constant is observed as the magnetic field is crossing the saturation value. At higher temperature, the jump is replaced by a minimum in the elastic constant. The minimal value of the elastic constant is an increasing function of $T$. We also note that the width of the region where the elastic constant decreases is larger as $T$ increases.

The specific heat is given by the derivative of the internal energy, $C_V = \frac{\partial U}{\partial T} = -\frac{1}{T^2} \left( \frac{\partial U}{\partial \beta} \right)$. Explicitly, the specific heat at constant volume is given by:

$$C_V(T, h) = -\frac{1}{T^2} \int \frac{dk}{2\pi} \frac{[\epsilon(k) - h]^2}{4 \cosh^2 \frac{\beta}{2} [\epsilon(k) - h]}.$$  

(81)

To calculate the specific heat at constant pressure, we derive the enthalpy $\mathcal{H}(t, \delta, h, p) = U(t, \delta, h) + p\delta$ and evaluate $C_p(T, p)$ as:

$$C_p = -\frac{1}{T^2} \int \frac{dk}{2\pi} \frac{[(1 - \delta)\epsilon(k) - h]^2}{4 \cosh^2 \frac{\beta}{2} [(1 - \delta)\epsilon(k) - h]} + \frac{1}{T^3} K - \frac{1}{T} \int \frac{dk}{2\pi} \frac{\epsilon(k)^2}{4 \cosh^2 \left( \frac{\beta}{2} \right)}.$$  

(82)

where the second part comes from the variation of $\delta$ with temperature. A plot of the specific heat is given on Fig. 14 for different temperatures. At very low-$T$ the specific heat presents a singularity that is replaced by a maximum at finite temperature.

2. Dilatation coefficient

We use the definition of the dilatation coefficient $\tau_S$, and Eq. (11) to obtain:

$$\alpha = \frac{1}{T^2} K - \frac{1}{T} \int \frac{dk}{2\pi} \frac{\epsilon(k)^2}{4 \cosh^2 \left( \frac{\beta}{2} \right)}.$$  

(83)
V. CONCLUSIONS

In this paper, we have discussed magnetostriction in an array of XX spin chains coupled to three dimensional acoustic phonons. We have shown that for low temperature, a first order transition would be obtained as a function of the magnetic field, with a jump of both the magnetization and the lattice constant. For higher temperatures, the discontinuity is replaced by a crossover, but anomalies are still visible in the elastic constant, the specific heat, the dilatation coefficient and the magnetic susceptibility. As we have explained in the introduction, our results are also relevant to ladder systems under magnetic field since the latter can be mapped in the limit of strong rung coupling onto XXZ chain model under field. We stress again the important differences between magnetostriction and the generalized spin Peierls transition of Ref. 37. First, in the generalized spin Peierls transition, a static lattice deformation of wavevector $q = 2\pi M$ where $M$ is the magnetization is expected. This would lead to extra reflections in an X-Ray scattering experiment. On the contrary, in magnetostriction, no superlattice is formed, and no new reflections are expected. Second, in the generalized spin Peierls transition, a spin gap is formed, leading to an exponential suppression of the specific heat and magnetic susceptibility at low temperature. In the case of magnetostriction, no spin gap is formed, leading to a $T$ linear specific heat and a finite susceptibility at low temperature in the partially magnetized phase. Also, in the case of the magnetostriction, anomalies are expected in the elastic constant and the dilatation coefficient as a function of the magnetic field. Of course, in a real system, both optical and acoustic phonons are present, and one should expect a coexistence of magnetostriction and generalized spin-Peierls effects. However, the first order transition under applied field is observable at higher temperature than the spin-Peierls transition so that the two effects can be separated in principle. It would be interesting to analyze the more general case of magnetostriction effects in a XXZ chain by using the TBA or by using Quantum Monte Carlo method. We expect that the general conclusions concerning the existence of the magnetostriction effect and the possibility to separate it from
FIG. 15: Dilatation coefficient for $T = 0.01, 0.03, 0.05$ for $P = 0$ and $K = J = 1$ as a function of the magnetic field. The dilatation coefficient vanishes in the fully polarized phase, and is negative in the partially polarized phase. We notice that the dilatation coefficient decreases strongly as temperature is increased. The behavior of the dilatation coefficient is non-monotonous as a function of the magnetic field.

the spin-Peierls transition will not be affected, and a more quantitative agreement with experiments will obtain. A more interesting extension of the present work would be to consider a two dimensional system of hard bosons coupled to phonons as this is relevant to the experiments on the TlCuCl$_3$ material$^{33}$ and the CuHpCl material$^{19}$. In two dimensions, hard bosons on a lattice can be mapped onto fermions in a gauge field$^{60,61}$. For a low fermion density, the corresponding gauge field is small. Therefore, at low magnetization, it can be expected that one can describe magnetostriction effect in a manner similar to the 1D case. We will leave this for future work.

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CALCULATION OF THE FIELD $h_{c2}$

The Eq. (20) can be rewritten as:

$$ P(\delta) = \left[ \pi^2 (K \delta + p)^2 - J^2 \right] (1 - \delta)^2 = h^2 $$

The extrema of the function $P$ are given by $dP/(d\delta) = 0$ i.e.:

$$ 2(\delta - 1) \left\{ \delta^2 + (3p/K - 1)\delta + \left[ \frac{p}{K} \right]^2 - \frac{p}{K} - \left( \frac{J}{\pi K} \right)^2 \right\} = 0, $$

(85)
giving a maximum for $\delta = \delta^+_c$, with:

$$ \delta^+_c = \frac{1}{4} \left[ 1 - \frac{3p}{K} + \sqrt{\left( 1 + \frac{p}{K} \right)^2 + 8 \left( \frac{J}{\pi K} \right)^2} \right] $$

(86)
and a minimum for $\delta = \delta_-$, with:
\[
\delta_- = \frac{1}{4} \left[ 1 - \frac{3p}{K} - \sqrt{\left(1 + \frac{p}{K}\right)^2 + 8 \left(\frac{J}{\pi K}\right)^2} \right]
\] (87)

The critical field $h_{c_\delta}$ is obtained by solving simultaneously the equation:
\[
P(\delta_-) = h_{c_\delta}^2
\] (88)

This is done by introducing the polynomial:
\[
\tilde{P}(\delta) = \delta^2 + (3p/K - 1)\delta + \left[\left(\frac{p}{K}\right)^2 - \frac{p}{K} - \left(\frac{J}{\pi K}\right)^2\right]
\] (89)

and writing $P(\delta) - h_{c_\delta}^2 = Q(\delta)\tilde{P}(\delta) + R(\delta)$. Since $P(\delta_-) = h_{c_\delta}^2$ and $\tilde{P}(\delta_-) = 0$, the equation is reduced to $R(\delta_-) = 0$. Since $R$ is a polynomial of degree 1, such an equation is trivial to solve. This leads to Eq. (22).
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