CBPF-NF-026/81

STRUCTURAL LIFSHITZ POINT IN THE QUASI D = 1 MAGNETOSTRICTIVE XY MODEL

by

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ABSTRACT

We obtain , within a fromework in which the crystalline degrees of freedom (assumed essentially three-dimensional) are adiabatically treated and the magnetic degrees of freedom are exactly (approximatively) treated in the disordered (ordered) phase (s), the peculiar phase diagram of the d = 1 first-neighbour spin - $\frac{1}{2}$ magnetostrictive XY model in the presence of a magnetic field along the Z-axis. The structural instability wave vector continuosly varies along the (2^{nd} order) critical line. This variation presents two non trivial points: one of them corresponds, in the phase diagram, to a Lifshitz point, where the uniform and dimerized phases converge with a (complex) modulated one; the other one presents characteristics which, to the best of our knowledge, have never been observed.

The problematics of commensurate/incommensurate long range orders and related phase transitions are being intensively studied nowadays (see Refs. [1-4] and references therein). The existence, in the associated phase diagrams, of Lifshitz multicritical points (LP) is clearly quite plausible, and has in fact been observed both theoretically[2,5-8] and experimentally[9] in magnetically ordered systems; in what concerns structurally ordered systems an experimental indication already exist[10]. In the present paper we exhibit a structural LP (associated with spin-Peierls instabilities). The system we discuss is the d = 1 first-neigbour spin - $\frac{1}{2}$ magnetostrictive XY (ferro or antiferromagnetic) model in the presence of a magnetic field (noted H) along the Z-axis: the exchange coupling constant and the elastic contribution are assumed to depend only on the mean positions of the spins (adiabatic approximation[11]; see also[12]), which is an approximate manner for taking into account the crystalline three-dimensionality of real substances (like TTF-BDT and alkali-TCNQ salts[9,13]); furthermore no soliton type structural defects are included within the present description; on the other hand the magnetic degrees of freedom are treated on perturbative grounds (nevertheless it will become clear further on that the present treatment remains exact in the disordered phase, i.e. uniform chaim; in particular the 2nd order phase boundary to be exhibited is the exact one as long as the magnetic degrees of freedom are concerned). Some aspects of this model have already been studied[14-17] but it will becomes clear herein that the most striking facts about the influence of the magnetic field were only partially revealed by previous work[15]; the same remark holds for a related model namely the Heisenberg one[12].

The magnetic contribution to the Hamiltonian of our system (cyclic linear chain with unitary fixed crystalline parameter) is given by

$$\mathcal{H}_m = - \sum_{j=1}^{2N} J_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) - \mu H \sum_{j=1}^{2N} S_j^z \tag{1}$$

where μ is the elementary magneton and we have considered 2N spins to facilitate comparisons with dimerized situations. Through the standard Jordan-Wigner transformation this Hamiltonian becomes

$$\mathcal{H}_m = - \frac{1}{2} \sum_{j=1}^{2N} J_j (a_j^+ a_{j+1} + a_{j+1}^+ a_j) - \mu H \sum_{j=1}^{2N} a_j^+ a_j + N\mu H \tag{2}$$

where the pseudo-fermion creation and annihilation operators have been introduced. Furthermore through Fourier transformation we obtain (by disregarding the term $N\mu H$)

$$\mathcal{H}_m = \mathcal{H}_0 + V \tag{3}$$

where

$$\mathcal{H}_0 = |J_0| \sum_{-\pi < k \leq \pi} \varepsilon_k a_k^+ a_k \tag{4}$$

and

$$V = \sum_{q \neq 0} \sum_k \Lambda_{kq} a_k^+ a_{k-q} \tag{5}$$

with

$$\varepsilon_k \equiv h - \cos k \tag{6}$$

$$h \equiv \mu H/|J_0| \tag{7}$$

$$\Lambda_{kq} \equiv \frac{1}{2} J_q [e^{-i(k-q)} + e^{ik}] \tag{8}$$

$$J_q \equiv \frac{1}{2N} \sum_{j=1}^{2N} e^{ijq} J_j \qquad (-\pi < q \leq \pi) \tag{9}$$

The magnetic field plays the role of the fermionic chemical potential [18]. Following along the lines of Ref. [16] we treat now V as a perturbation (up to the second order) within the temperature dependent Green functions framework, we include the elastic term $\sum_{j=1}^{2N} \frac{C}{2} (X_{j+1}-X_j)^2$ ($\{X_j\}$ being the spin positions with respect to the uniform chain equilibrium ones), and we expand $J_j = J(0) + J'(0)(X_{j+1}-X_j)$ ($J(0) = J_0$ and $J'(0)$ being positive or negative constants). We finally arrive to

$$f = f_0 + \frac{1}{2} \sum_{q\neq 0} \omega_q^2 \eta_q^2 + K\eta_0^2 \tag{10}$$

where

$$f_0 \equiv \frac{F_0}{N|J_0|} = -\frac{2t}{\pi} \int_0^{\pi} dk \; \ell n \; 2 \; ch \frac{\varepsilon_k}{2t} \tag{11}$$

and $f \equiv F/N|J_0|$ are respectively the magnetic uniform chain and total modulated chain reduced free energies (we have used the quasi-continuum limit), and where

$$\omega_q^2 \equiv (1-\cos q) \left\{ K - \frac{1}{4\pi \sin\frac{q}{2}} \int_0^{\pi} dk \frac{\cos^2 k}{\sin k} \left[th \frac{\varepsilon_{k+q/2}}{2t} - th \frac{\varepsilon_{k-q/2}}{2t} \right] \right\} \tag{12}$$

$$\eta_q \equiv 2\left|\frac{J'(0)}{J(0)}\right| |X_q| \qquad (13)$$

(X_q being the Fourier transform of X_j)

$$K \equiv C|J_0|/|J'(0)|^2 \qquad (14)$$

$$t \equiv k_B T/|J_0| \qquad (15)$$

The critical frontier in the t,h,K - space wich separates the uniform (U) phase from the dimerized (D) and modulated (M; higher order commensurate or incommensurate modulations) ones is determined, as long as it refers to second order phase transitions (and we have verified in several typical situations that this is indeed the case), by $\omega_{q_c}(t,h,K) = 0$ where q_c is the wave vector of the structural mode which first becomes unstable (coming from the U phase): see Fig. 1 (see also Refs.[15,16]). Through this criterium we have obtained the phase diagram reproduced in Fig.2 where the dashed curves refer to iso-q_c lines (for different values of the reduced elastic constant K). For $K < K^* \simeq 0.2$ it is possible to have, for fixed t and increasing h, the sequence $\eta_q \neq 0$, $\eta_q = 0$, $\eta_q \neq 0$ and $\eta_q = 0$; this remarkable possibility disappears for $K > K^*$, and it is striking the fact that at precisely the value K^* occurs[17] a changement in the t-γ phase diagram where γ is an XY coupling anisotropy (in the present model γ vanishes). We remark that, for a given value of K, two special points (inflexion ones) appear in the the t-h diagram, respectively corresponding to $q_c = \pi$ and $q_c = 0$; the former corresponds to a Lifshitz point; the latter is the starting point above which q_c vanishes, following along the critical line towards the universal point ($t=0$; $h=1$). In order to better understand the $q_c = 0$ starting point we have discussed the exact free energies (no small η_q expansions) associated to $q_c = 2\pi/s$ with $s = 2,3,4$ (respectively associated with the dimerized, trimerized and tetramerized configurations; sinuisodal long range order has been considered) and our results are illustrated, for $K = 0.4$, in Fig.3: three phases are present (namely the U, D and M ones) which join at the LP; the D-M phase boundary is a first order one (the metastability lines (dashed) are indicated as well) while the U-D and U-M critical lines correspond to second order (or continuous) phase transitions; the iso-q lines (dotted; do not confuse with the iso-q_c lines of Fig. 2) associated with $q = 2\pi/3$ and $q = \pi/2$ are indicated as well. One can speculate that the iso-q line for $q \to 0$ coalesces with that part of the U-M critical line above the starting point associated with $q_c = 0$.

We intend to publish elsewhere full details concerning the present discussion as well as the thermal and magnetic field dependences of quantities such as dimerized order parameter, specific heat, magnetic isothermal susceptibility, $q = 0$ optic mode frequency, sound velocity and external stress effects.

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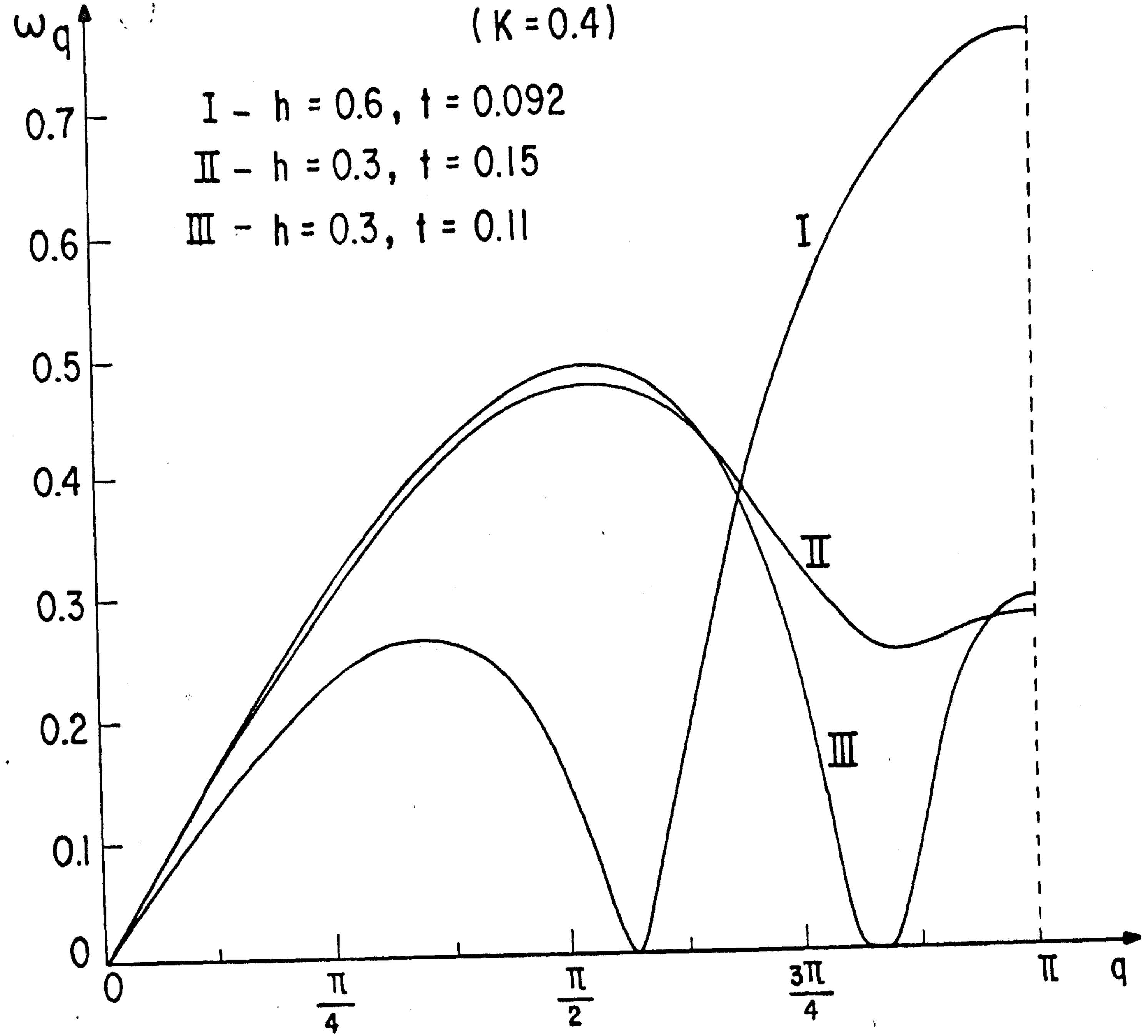
CAPTION FOR FIGURES

Fig. 1 - Spectra associated, for fixed temperature, magnetic field, and elastic constant, with frozen structures characterized by wave vectors q. The cases I and III (but not II) exhibit the trigger of incommensurate (or high-order commensurate) macroscopic instabilities.

Fig. 2 - Temperature - magnetic field 2nd order critical (continuous) and iso-q_c (dashed) lines associated with different elastic constants K. The iso-q_c line for $q_c=\pi$ ($q_c= 0$) is a Lifshitz ("starting") one.

Fig. 3 - The K = 0.4 phase diagram. On the Lifshitz point (LP) converge the uniform (U), dimerized (D) and (complex) modulated (M) phases. The continuous (dot-dashed) line is a second (first) order phase transition one; the dashed lines are metastability ones; the dotted lines are the iso-q (do not confuse with iso-q_c) ones associated with $q = 2\pi/3$ and $q = \pi/2$ (respectively trimerized and tetramerized structures) and they are tangential to the U-M critical line.



ωq
(K = 0.4)
I - h = 0.6, t = 0.092
II - h = 0.3, t = 0.15
III - h = 0.3, t = 0.11
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
I
II
III
0
π/4
π/2
3π/4
π
q

FIG.1

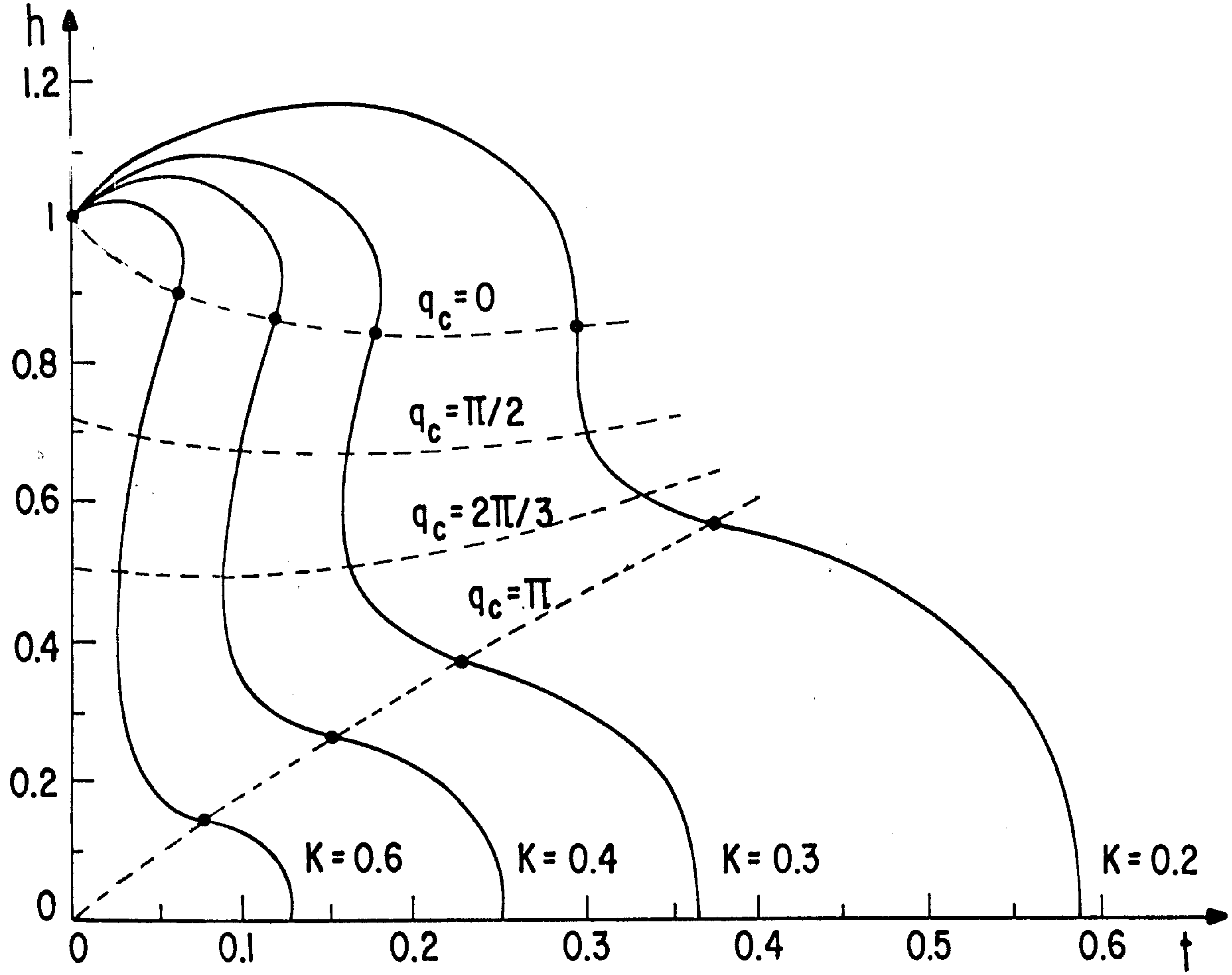

h
1.2
1
0.8
0.6
0.4
0.2
0
q_c = 0
q_c = π/2
q_c = 2π/3
q_c = π
K = 0.6
K = 0.4
K = 0.3
K = 0.2
0
0.1
0.2
0.3
0.4
0.5
0.6
t

FIG. 2

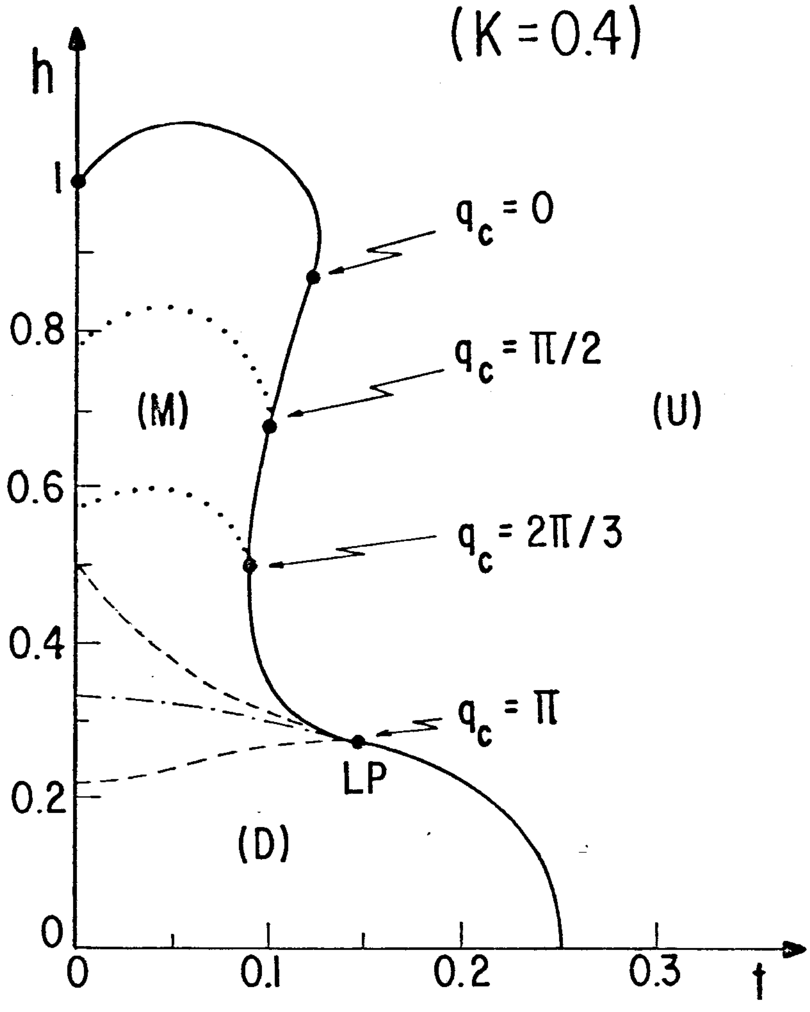


FIG.3