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Phase Diagram of a Spin-1 Quantum Ising Model with Dipole and Quadrupole Interactions

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A quantum Ising-like spin-1 system with both dipole and quadrupole interactions is analyzed. Such model is a generalized quantum version of the Blume-Emery-Griffiths model in an external anisotropic field. Models of this type are interesting candidates to describe phase transitions in liquid crystals. The phase diagram as well as the thermodynamic potentials of the model are constructed by a recently formulated improved version of mean field theory.

The latter, which has the usual mean field theory as its zero-th order approximation, takes into account fluctuations up to the fourth-order. The phase diagram is found to exhibit phase transition manifolds of both the first and the second order, as well as multicritical lines. Four phases can be recognized: one ferromagnetic and three paramagnetic. The phases are identified by the requirements of minimum free energy constrained by the condition of self consistency of the order parameters p and q.

INTRODUCTION

The formal transformation, whereby the Lee-Yang lattice gas model[1] maps into a pseudo-spin Ising-like model, has been widely exploited to describe cooperative phenomena in both fluids and liquid crystals. The latter are indeed more clearly understandable in terms of ordering of the spin system for which the order parameter has a direct intuitive meaning.

Whereas great attention has been devoted to the spin ½ case, the higher spin models have been somewhat neglected, even though they seem to be able to exhibit promising features, especially in the application to liquid crystal and liquid crystal mixtures.

The relevant property for this is that they are characterized by more than one order parameter. For example in a spin 1 model there are two order

parameters, that are not independent and give rise to a rich structure of the phase space, due to the mutual interaction between the two ordering processes they represent.

Consider as an example a mixture, one of whose two components consists of elongated molecules which can assume only two orientations and is hence characterized by some cooperative ordering (such as that ordinarily described by the spin-½ Ising model); whereas, the other component, made up of spherical molecules, is insensitive to such cooperative phenomenon and hinders the nematic phase transition. The spin-1 model will then describe the dilution effect on the nematic ordering as well as the phase separation induced in the isotropic fluid both by the intermolecular forces and by the driving nematic ordering itself.

Pioneering work along these lines was done by Lajzerowicz and Sivardière[2] who considered a spin-1 lattice gas model characterized by an Ising-like Hamiltonian similar to the Blume-Emery-Griffith model.[3] The same type of model was more recently studied by Gefen, Imry and Mukamel,[4] who besides the usual dipolar and quadrupolar interactions included in the model the coupling with a transverse field.

The latter authors also analyzed the critical behavior of the system by real-space renormalization group techniques.

The results concerning the phase diagram structure (including the order of the transitions and the multicritical points) are generally found to be in good quantitative agreement with conventional mean-field theory for isotropic $d \geqslant 2$ dimensional models.

However, if the system exhibits anisotropies, the fluctuations of the order parameters are so wide that the results of ordinary mean field theory cease to be correct, in some instances even qualitatively.

The origin of such failure has been thoroughly studied recently,[5–8] and can be ascribed on the one hand to the intrinsic limitations of the molecular-field approximation, which is unable to take into account any many-body correlation effect, on the other hand to the ambiguity in the adoption of a consistency condition for the theory.

In this paper the study of a quantum spin-1 Ising-like system with dipole and quadrupole interactions in an external anisotropic field is approached by a recently formulated improved version of mean field theory.[8,9]

The latter, which has the ordinary mean field theory as its zero-th order approximation, takes into account spin-fluctuations in the cluster expansion of the free energy, up to the fourth order.

In Section I together with the model Hamiltonian, are briefly described both the procedure whereby the latter is factorized, and the derivation — within the framework of the above theory — of the zero temperature general form of the free energy.

In Section II the consistency equations are discussed, as well as the phase diagram they lead to. The latter has been chosen to represent the two order parameters, expressing the thermal average of the z-components of both the dipole and the (diagonal) quadrupole operators vs the model parameters. Such a diagram is found to exhibit a very rich structure in which one recognizes phase transition manifolds of both the first and the second order, as well as multicritical lines. Four phases can be recognized, one ferromagnetic and three (inequivalent) paramagnetic. The numerical results are discussed and compared with those of Refs. 2 and 4 (which are recovered here simply by the zero-th order treatment). In Section III as a conclusion the possibilities of application of the model are discussed, together with the possible extension—in a few particularly significant cases—of the phase diagram, by addition of the temperature as a state variable.

I. The Model Hamiltonian and Free Energy

The model Hamiltonian reads

$$H = \sum_{i=1}^{N} \{B_x S_i^{(x)} + B_z S_i^{(z)} + D_x Q_i^{(x)} + D_z Q_i^{(z)}\} - \frac{1}{2} \sum_{j,k=1}^{N} \{J_{jk} S_j^{(z)} S_k^{(z)} + G_{jk} Q_j^{(z)} Q_k^{(z)}\} \tag{1.1}$$

where $S_i^{(\alpha)}$, $Q_i^{(\alpha)}$, $\alpha = x, z$ are respectively dipole (vector) and quadrupole (tensor) operators at site i, $i = 1, \ldots, N$ of a d-dimensional ($d \geqslant 2$) lattice, B_α are the components of an external field and D_α the anisotropy exchange interactions. In a representation in which single particle operators are written as rank 3 matrices,

$$S_i^{(\alpha)} = I_3 \otimes I_3 \otimes \ldots \otimes S^{(\alpha)} \otimes I_3 \otimes \ldots \otimes I_3 \tag{1.2}$$

$$Q_i^{(\alpha,\gamma)} = I_3 \otimes I_3 \otimes \ldots \otimes S^{(\alpha)} S^{(\gamma)} \otimes I_3 \otimes \ldots \otimes I_3 \tag{1.3}$$

$$Q_i^{(\alpha)} \triangleq Q_i^{(\alpha,\alpha)} \tag{1.4}$$

The operators $S^{(\alpha)}$ are the components of the spin-1 vector operator in the customary rank-3 matrix representation

$$S^{(x)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \qquad S^{(z)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{1.5}$$

they enter in the N-terms tensor product at the r.h.s. of Eqs. 1.2 and 1.3 at the i-th position.

Upon introduction of the spin-fluctuation operators

$$\delta S_i^{(z)} = S_i^{(z)} - p; \qquad \delta Q_i^{(z)} = Q_i^{(z)} - q \tag{1.6}$$

where p, q are real numbers, such that $\|\delta S_i^{(z)}\| \ll p$, $\|\delta Q_i^{(z)}\| \ll q$; $\|\cdot\|$ denoting a suitable norm; the Hamiltonian H can be factorized in the form

$$H = H_0 + H' \tag{1.7}$$

where H' is the part bilinear in both $\delta S_i^{(z)}$ and $\delta Q_i^{(z)}$:

$$\begin{aligned} H' &\triangleq -\frac{1}{2}\sum_{j,k=1}^{N}\left\{J_{jk}\delta S_j^{(z)}\delta S_k^{(z)} + G_{jk}\delta Q_j^{(z)}\delta Q_k^{(z)}\right\} \\ &= -\frac{1}{2}\sum_{j,k=1}^{N}\left\{J_{jk}S_j^{(z)}S_k^{(z)} + G_{jk}Q_j^{(z)}Q_k^{(z)} - pJ_{jk}(S_j^{(z)} + S_k^{(z)})\right. \\ &\qquad \left. -qG_{jk}(Q_j^{(z)} + Q_k^{(z)}) + p^2J_{jk} + q^2G_{jk}\right\} \\ &= \sum_{j,k=1}^{N} H'_{jk} \end{aligned} \tag{1.8}$$

H'_{jk} are two particle operators.

$$H_0 = \sum_{i=1}^{N}\left\{L + B_xS_i^{(x)} + MS_i^{(z)} + D_xQ_i^{(x)} + VQ_i^{(z)}\right\} = \sum_{i=1}^{N} H_{0i} \tag{1.9}$$

with

$$L = \frac{1}{2}(p^2\mathcal{J} + q^2\mathcal{G}), \qquad M = B_z - p\mathcal{J}, \qquad V = D_z - q\mathcal{G},$$

$$\mathcal{J} = \sum_k J_{jk}, \qquad \mathcal{G} = \sum_k G_{jk}$$

We will confine henceforth our attention to the case of nearest-neighbor (n.n.) coupling

$$J_{jk} = \begin{cases} J \\ 0; \end{cases} \qquad G_{jk} = \begin{cases} G & \text{if } (j,k) = \text{n.n.} \\ 0 & \text{otherwise} \end{cases}$$

In this case $\mathcal{J} = zJ$, $\mathcal{G} = zG$, z denoting the number of n.n. per site. The factorization Eq. 1.7 is the starting point for the adoption of a generalized version of the mean field theory — thoroughly discussed in Refs. 6–8 — whereby, through the use of an explicit form of the inverse Baker — Campbell — Hausdorff formula, and a consistent combination of cumulant and cluster expansions, the free energy

$$F = -\frac{1}{\beta} \ln Tr\{\exp(-\beta H)\} \tag{1.10}$$

can be written in a form including the effect of fluctuations up to the fourth order. In present application the results referred to above lead to

$$F = F_0 + F' \tag{1.11}$$

where

$$F_0 = -\frac{1}{\beta} \ln Tr\{\exp(-\beta H_0)\},$$

whereas

$$F' = \frac{Nz}{2} \exp\left(2\beta \frac{F_0}{N}\right) \left\{T_1 - \beta T_2 + \beta \exp\left(2\beta \frac{F_0}{N}\right) \cdot \left[\frac{Nz}{2} T_1^2 - P_2\right]\right\} \tag{1.12}$$

In Eq. 1.12 the quantities T_1, T_2 and P_2 are related to the expectation values in the unperturbed state determined by H_0, of the two body part of the Hamiltonian, H'. In terms of the rank-9 matrix

$$\begin{aligned}\mathcal{H}' = &-JS^{(z)} \otimes S^{(z)} - GQ^{(z)} \otimes Q^{(z)} + pJ(S^{(z)} \otimes I_3 + I_3 \otimes S^{(z)}) \\ &+ qG(Q^{(z)} \otimes I_3 + I_3 \otimes Q^{(z)}) - (Jp^2 + Gq^2)I_9\end{aligned} \tag{1.13}$$

they read,

$$T_1 = \sum_{a=1}^{9} \exp(-\beta E_a) \langle \nu_a | \mathcal{H}' | \nu_a \rangle \tag{1.14}$$

$$T_2 = \sum_{a=1}^{9} \sum_{c=1}^{9} \exp(-\beta E_a) L[\beta(E_a - E_c)] |\langle \nu_a | \mathcal{H}' | \nu_c \rangle|^2 \tag{1.15}$$

$$\begin{aligned}P_2 = &\sum_{A=1}^{81} \sum_{B=1}^{81} \exp(-\beta \mathcal{E}_A) L[\beta(\mathcal{E}_A - \mathcal{E}_B)] \langle \mu_A | \mathcal{H}' \otimes I_9 | \mu_B \rangle \\ &\cdot \left\{2(z-1) \langle \mu_B | I_3 \otimes \mathcal{H}' \otimes I_3 | \mu_A \rangle \right. \\ &\left. + \left(\frac{Nz}{2} - 2z + 1\right) \langle \mu_B | I_9 \otimes \mathcal{H}' | \mu_A \rangle \right\}\end{aligned} \tag{1.16}$$

The symbols in Eqs. 1.14 to 1.16 have the following definitions. The function L is given by

$$L(x) = \frac{\sinh x - x}{x^2} + \frac{\cosh x - 1}{x^2} \tag{1.17}$$

Moreover, upon denoting by $\mathcal{H}_0$ the 3×3 matrix

$$\mathcal{H}_0 = LI_3 + B_x S^{(x)} + MS^{(z)} + D_x Q^{(x)} + VQ^{(z)} \tag{1.18}$$

by R the orthogonal rotation matrix which diagonalizes $\mathcal{H}_0$,

$$R^{-1}\mathcal{H}_0 R = \{\text{diag } \varepsilon_\alpha;\ \alpha = 1, 2, 3\} \tag{1.19}$$

and by $\{|\eta_\alpha\rangle\}$ the eigenkets of $\mathcal{H}_0$; we introduce the rank 9 matrices

$$\mathcal{H}_0^{(2)} = \mathcal{H}_0 \otimes I_3 + I_3 \otimes \mathcal{H}_0 \tag{1.20}$$

$$R_2 = R \otimes R \tag{1.21}$$

and the rank 81 matrices

$$\mathcal{H}_0^{(4)} = \mathcal{H}_0^{(2)} \otimes I_9 + I_9 \otimes \mathcal{H}_0^{(2)} \tag{1.22}$$

and

$$R_4 = R_2 \otimes R_2 \tag{1.23}$$

then

$$R_2^{-1}\mathcal{H}_0^{(2)}R_2 = \{\text{diag } E_a;\ a = 1, \ldots, 9\};$$
$$E_a = \varepsilon_\alpha + \varepsilon_\beta; \qquad (\alpha, \beta) \leftrightarrow a \tag{1.24}$$
$$R_4^{-1}\mathcal{H}_0^{(4)}R_4 = \{\text{diag } \mathcal{E}_A;\ A = 1, \ldots, 81\};$$
$$\mathcal{E}_A = E_a + E_b; \qquad (a, b) \leftrightarrow A \tag{1.25}$$

and the eigenkets are $\{|\nu_a\rangle = |\eta_\alpha\rangle|\eta_\beta\rangle\}$ for $\mathcal{H}_0^{(2)}$ and $\{|\mu_A\rangle = |\nu_a\rangle|\nu_b\rangle\}$ for $\mathcal{H}_0^{(4)}$ respectively.

In present application we aim to discuss the structure of the phase diagram and restrict therefore our attention to the zero temperature ($\beta \to \infty$) value of F. The evaluation of the latter is nontrivial, and requires a lengthy algebraic manipulation. We sketch here only the relevant steps, leaving the details to a further paper, where the group—theoretical structure of the whole procedure will be clarified.

Let us introduce first a basis $\{X_a;\ a = 0, \ldots, 8\}$ for the ring of rank 3 matrices. We select the X_a's in such a way that $X_0 = \sqrt{2/3}\, I_3$ and

$$Tr\{X_a\} = 0 \qquad a = 1, \ldots, 8 \tag{1.26}$$

With such a choice, any 3×3 matrix $M \equiv \{m_{ij} | i, j = 1, 2, 3\}$ can be written as

$$M = \sum_{a=0}^{8} \mu_a X_a \tag{1.27}$$

with

$$\mu_a = \frac{1}{2} Tr\{MX_a^T\} \tag{1.28}$$

In the basis in which $\mathcal{H}_0^{(2)}$ is diagonal, $\mathcal{H}'$ assumes the form

$$R_2^{-1}\mathcal{H}'R_2 = \sum_{r=1}^{3}\sum_{j=1}^{3} h_{rj} X_r \otimes X_j \tag{1.29}$$

or, explicitly,

$$\langle \nu_a|\mathcal{H}'|\nu_b\rangle = \sum_{r,j} h_{rj}(X_r)_{\alpha\beta}(X_j)_{\gamma\delta} = F^{\beta\delta}_{\alpha\gamma}, \qquad (\alpha,\gamma) \leftrightarrow a; \qquad (\beta,\delta) \leftrightarrow b \tag{1.30}$$

The $\{h_{rj}\}$ are straight forwardly derived from Eq. 1.13 by repeated application of Eqs. 1.27 and 1.28. Upon setting

$$\varepsilon_m = \min_{1\leqslant j\leqslant 3}\{\varepsilon_j\} \tag{1.31}$$

we can finally write

$$\lim_{\beta\to\infty}\frac{F}{N} = f_0 = \varepsilon_m + \frac{1}{2}zF^{mm}_{mm} + \frac{1}{2}z\sum_{c\neq m}\sum_{d\neq m}\frac{F^{cd}_{mm}F^{mm}_{dc}}{2\varepsilon_m - \varepsilon_c - \varepsilon_d} + z^2\sum_{d\neq m}\frac{F^{md}_{mm}F^{mm}_{dm}}{\varepsilon_m - \varepsilon_d} \tag{1.32}$$

A more explicit expression for f_0, valid in any regime determined by Eq. 1.31 and for generic spin will be given elsewhere.

II. Self-consistency and Phase Diagram

The ground state energy, as given by Eq. 1.32 is naturally a function of both the set of parameters $P \equiv \{B_x, B_z, D_x, D_z, J, G\}$ and the two order parameters p and q; $f_0 = f(P; p, q)$.

In what follows we shall drop the argument P in f, whenever no ambiguity arises.

The equilibrium value of latter should be computed from a self-consistency condition of the theory. It has been a matter of long speculations,[5,8] yet not completely settled, that the two "natural" conditions one can think of, namely: (i) that at equilibrium the free energy be

minimum; (ii) that the order parameters represent the most probable value of the dynamical variable they refer to; are uncompatible with each other.

In present application, condition (i) would lead to the pair of equations

$$\frac{\partial f}{\partial p} = \frac{\partial f}{\partial q} = 0 \tag{2.1}$$

whose solutions $p = p_0(P)$, $q = q_0(P)$ are of course subjected to the further constraint that

$$\left.\frac{\partial^2 f}{\partial q^2}\right|_{q=q_0} > 0, \qquad \frac{\partial^2 f}{\partial q^2}\frac{\partial^2 f}{\partial p^2} - \left(\frac{\partial^2 f}{\partial p \partial q}\right)^2 \Bigg|_{\substack{p=p_0 \\ q=q_0}} > 0;$$

or are to be chosen in correspondence of the absolute minimum of f_0 in the range $|p| \leqslant 1$, $q \leqslant 1$ if this is lower than $f(p_0, q_0)$. Condition (ii) on the other hand would lead to

$$\langle S_i^{(z)} \rangle = p, \qquad \langle Q_i^{(z)} \rangle = q \tag{2.2}$$

where $\langle \Theta \rangle = (1/Z)\, Tr\{\Theta e^{-\beta H}\}$ denotes thermal average of any operator Θ. The l.h.s. of Eq. 2.2 are easily calculated observing that

$$\langle S_i^{(z)} \rangle = \frac{\partial f}{\partial B_z}; \qquad \langle Q_i^{(z)} \rangle = \frac{\partial f}{\partial D_z} \tag{2.2}$$

Eq. 2.2 requires that at equilibrium the thermal average of the fluctuations $\delta S_i^{(z)}$ and $\delta Q_i^{(z)}$ vanish. We expect their solutions $p = p_1(P)$, $q = q_1(P)$ to be more reliable, in that the latter requirement is more compatible with the structure of the whole theory, designed so as to keep into account fluctuations only up to finite order.

The ambiguity arises from the fact that $f(p_1, q_1)$ is not necessarily a minimum.

However, it turns out that the domain in the (p, q) plane where (p_1, q_1) is located, in most cases corresponds to a region of great stability of f_0, which is essentially flat there. On the other hand the domain in which (p_0, q_0) leads to values of $\langle \delta S_i^{(z)} \rangle$, $\langle \delta Q_i^{(z)} \rangle$ is extremely large, and therefore such that the very assumptions at the basis of the theory are violated, and its results (fourth order in the fluctuations) cannot be relayed upon.

Notice that at the order zero (which corresponds to the ordinary mean field theory) the ambiguity does not exist, because of the lack of correlation effects.

We adopt, therefore, the following procedure. Upon introducing the Lagrange multipliers λ, μ we define

$$U = U(p, q; \lambda, \mu) = f(p, q) + \mu(\langle S_i^{(z)} \rangle - p) + \lambda(\langle Q_i^{(z)} \rangle - q) \tag{2.3}$$

The minimization procedure, performed over U, gives the functions

$$p = \bar{p}(\lambda, \mu), \quad q = \bar{q}(\lambda, \mu) \tag{2.4}$$

Inserting the latter into Eqs. 2.2, λ and μ can be computed. If the multipliers turn out to be both of the order of $\|H'\|/\|H_0\|$, $\bar{p}$ and $\bar{q}$ are assumed as solutions, and their basins of attraction determine the phase diagram.

Several types of situation occur, separated by both first and second order transition lines and in some case by tricritical lines. The latter are to be determined by performing first a Landau expansion of f_0, $\langle S_i^{(z)} \rangle$ and $\langle Q_i^{(z)} \rangle$ in powers of p in Eq. 2.3, and then solving the stationarity equations for U for the first few terms in the expansion. The different critical lines and surfaces, which are thus represented parametrically, are given by the vanishing of the terms corresponding to the coefficients of increasing order in such truncated equations.

The analytic details of the above procedure will be reported elsewhere; here we will report only the numerical results, of particular interest for the application to the liquid crystal case, and discuss the relevant features.

In order to describe the results, we represent all the quantities in dimensionless units, such that $\mathcal{J} = 1$;

$$b_x = \frac{B_x}{\mathcal{J}}; \qquad d_x = \frac{D_x}{\mathcal{J}}; \qquad d_z = \frac{D_z}{\mathcal{J}}; \qquad g = \frac{G}{\mathcal{J}} \tag{2.5}$$

with the proviso that the case of pure quadrupolar interaction ($J = 0$) is not included in present discussion. The latter, which is a special case of a more general type of interaction will be discussed elsewhere in a more global framework. Moreover in present work, B_z is assumed to be zero: this does not affect the generality of the discussion, in that the effect of a parallel field would be only to smooth out the second order phase transition lines. Finally, the ground state stability requires that $g \geq 0$. Notice that for $g = 0$ the order parameter q need not be introduced, in that $\langle Q_i^{(z)} \rangle$ can be calculated explicitly as a function of p.

The several different choices performed of the parameters b_x and g will be presented in order of increasing complexity; emphasizing in each case the most relevant features. The first set of results refers to a zero-th order treatment of the model; the second set of results derives from the general theory discussed before.

(a) $b_x = 0$, order zero

In this case the phase diagram is represented in the (d_z, d_x) plane, by Fig. 1.

It exhibits four inequivalent phases, three of which are paramagnetic:

P_1, characterized by $p = 0$, $q = \langle Q_i^{(z)} \rangle = 1$

P_2, characterized by $p = 0$, $q = \langle Q_i^{(z)} \rangle = 0$

P_3, characterized by $p = 0$, $q = \langle Q_i^{(z)} \rangle = 1$

and one ferromagnetic:

F, characterized by

$$|p| = \sqrt{1 - \frac{d_x^2}{4}}, \qquad q = \langle Q_i^{(z)} \rangle = 1$$

The phases P_1 and P_3 differ by reversal of all the spin z-components. Phase F is separated from P_1 and P_3 by second order transition lines l_1 (of equation $d_x = 2$) and l_3 ($d_x = -2$) respectively, and from P_2 by a first order transition line l_2 ($d_z = (1/8)d_x^2 + (1/2)d_x + 1/2(g + 1)$). The paramagnetic phases are mutually separated by first order transition lines. P_1 and P_2 by the line l_{12} ($d_z = d_x + g/2$); P_2 and P_3 by the line l_{23} ($d_z = g/2$) respectively.

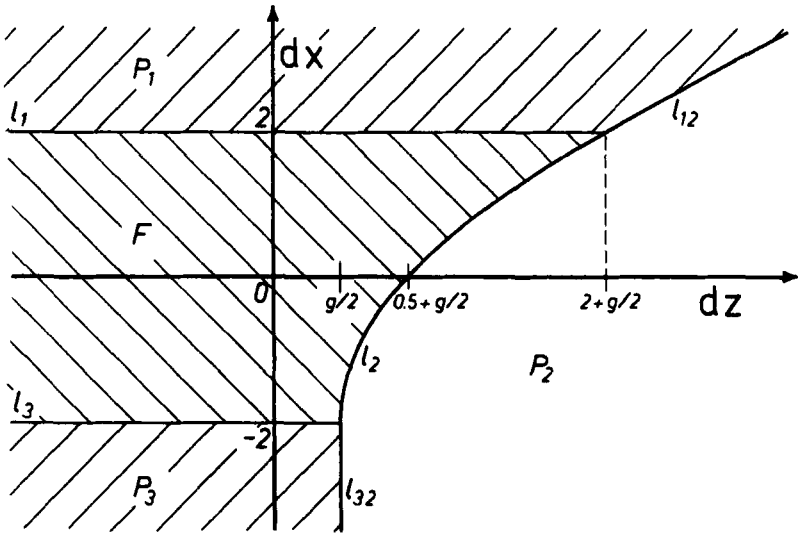

FIGURE 1 The zero-th order, phase diagram (d_z, d_x) for $b_x = 0$. The zones P_a, a = 1,2,3 represent the paramagnetic phases, F the ferromagnetic phase. The lines l_1, l_3 are second order transition lines; l_2, l_{12}, l_{32} are first order transition lines.

Notice how, in present case, switching on a value of g different from zero amounts simply to move rigidly the phase diagram of $g/2$ along the d_z axis.

(b) $b_x \neq 0$, order zero

This case was thoroughly discussed in Ref. 4, only for the $g = 0$ case. Moreover, in the same reference the case $g = 0$ was treated by the adoption of two order parameters, p and q. As we already pointed out, the latter in such case is not necessary, and a complete analytic discussion can be carried out in terms of p alone. $\langle Q_i^{(z)} \rangle$ is of course relevant to determine the phase portrait.

The phase diagram is now conveniently represented by the (d_z, d_x, b_x) space.

In Figure 2 the latter is described by a set of sections performed by a congruence of planes $d_z = \text{const}$. In such sections the resulting curves in the (d_x, b_x) plane describe the movement of the lines l_a, $a = 1, 2, 3$, and l_{1b}, $b = 2, 3$ (l_{23} disappears as b_x is switched on).

Two characteristic values of g, $g = 0$ and $g = 1$ are presented. It is interesting to notice how, for d_z varying from large negative values up to $\sim g/2$, the ferromagnetic phase F narrows more and more rapidly, and is shifted towards positive d_x as b_x increases from zero to large positive values.

As d_z varies between $g/2$ and $2 + g/2$, the surface issuing from the line l_2 of the $b_x = 0$ case, for $g = 0$ exhibits a splitting into two parts, the lower one (low b_x) corresponding to a first order phase transition which is the natural continuation of the $b_x = 0$ case; the upper one (large b_x) describing a second order transition. The two parts are separated by a line of tricritical points t.

As d_x grows beyond $2 + g/2$, t merges to a point on the $b_x = 0$ plane, and we have an interesting feature. For $g = 0$ the surface issuing from l_{12} bifurcates in two sheets which enclose a ferromagnetic phase, both representing a second order transition.

For $g \neq 0$ the surface, unique for low b_x, bifurcates — again at a tricritical line — for finite b_x into two sheets, one describing first order, the other one second order transitions.

Thus for b_x large enough, the system exhibits a ferromagnetic phase at points in the (d_z, d_x) plane which in Figure 1 are purely paramagnetic. Figures 3, 4 and 5, show the behavior of p and $\langle Q_i^{(z)} \rangle$ vs d_x for $g = 0$, $d_z = -1$ and $d_z = 1$, and of p and q vs d_x for $g = 1$, $d_z = 1$ respectively.

The above choices of parameters characterize the relevant physical situations.

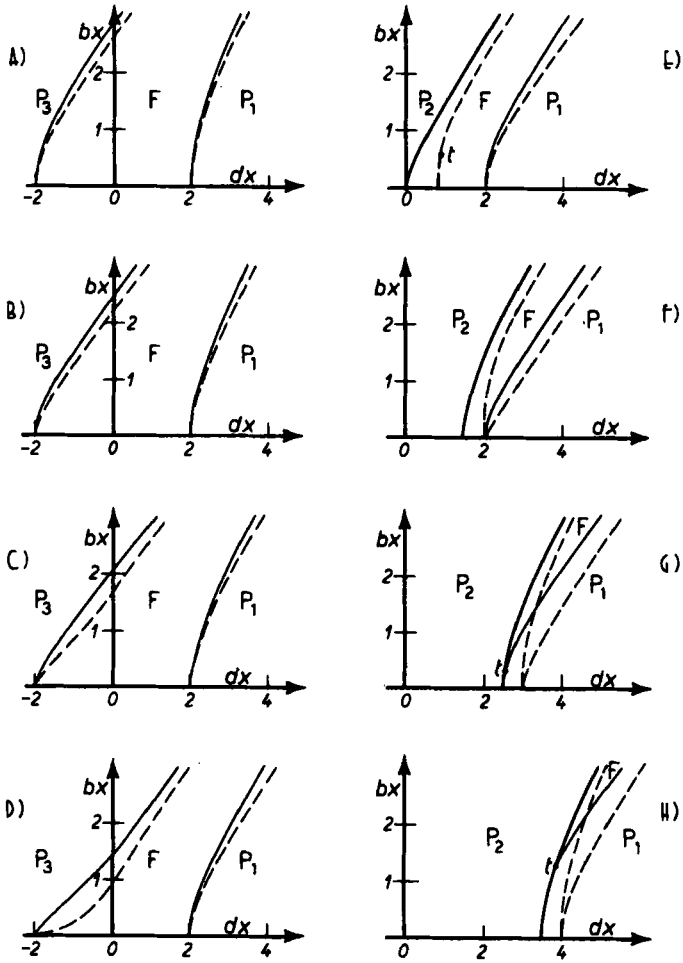

FIGURE 2 The zero-th order phase diagram (d_z, d_x, b_x): (A) $d_z = -3$, (B) $d_z = -2$, (C) $d_z = -1$, (D) $d_z = 0$, (E) $d_z = 1$, (F) $d_z = 2$, (G) $d_z = 3$, (H) $d_z = 4$. The phases are indicated by the same symbols as in Figure 1). Broken lines correspond to $g = 0$, full lines to $g = 1$. Thick lines indicate first order transitions, thin lines second order transitions. t denotes tricritical point.

(c) $b_x = 0$, second order

The procedure described in Sect. I introduces significant corrections for both the phase diagram and the behavior of the polarization p. Figure 6 shows p vs $|d_x|$ (the function is even in d_x) for different choices of the coordination number z; comparing it with the zero-th order result (which

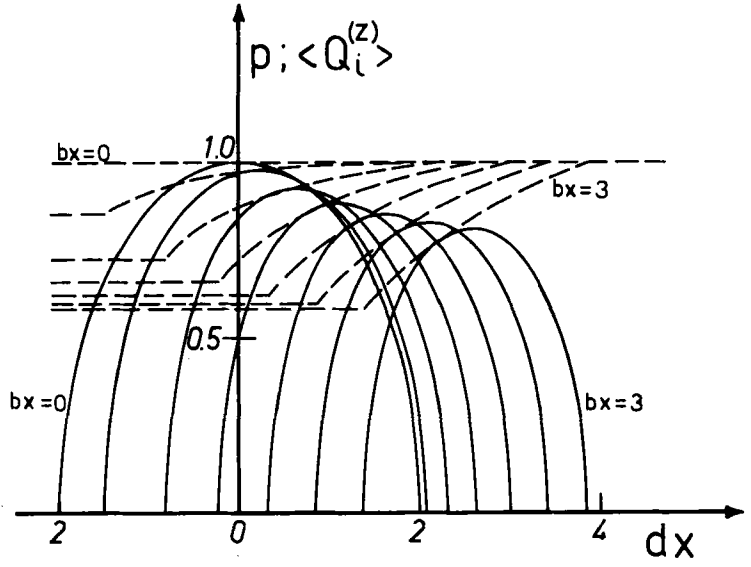

FIGURE 3 The order parameter p (full lines), and the quadrupole operator thermal average $\langle Q_i^{(z)} \rangle$ (broken lines) vs d_x for $g = 0$, $d_z = -1$ and b_x ranging from 0 to 3 (step 0.5).

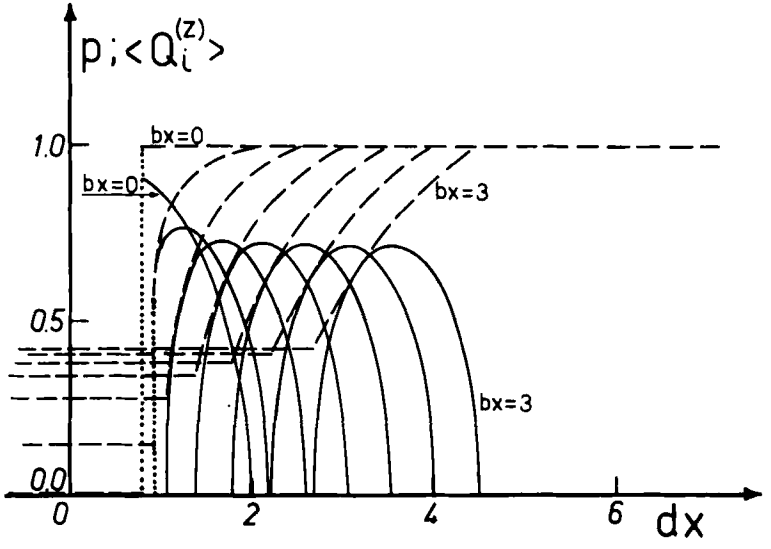

FIGURE 4 Same as Figure 3, for $g = 0$, $d_z = 1$.

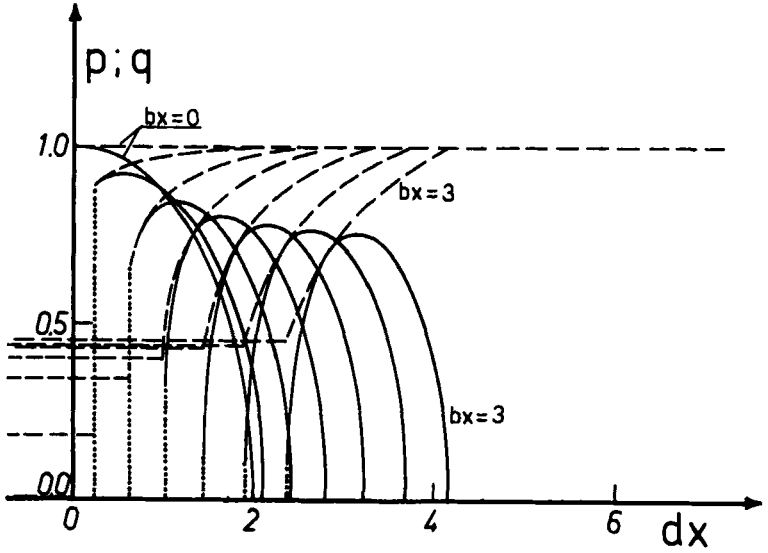

FIGURE 5 The order parameters p (full line) and q (broken line) vs d_x for $g = 1$, $d_z = 1$ and b_x ranging from 0 to 3 (step 0.5).

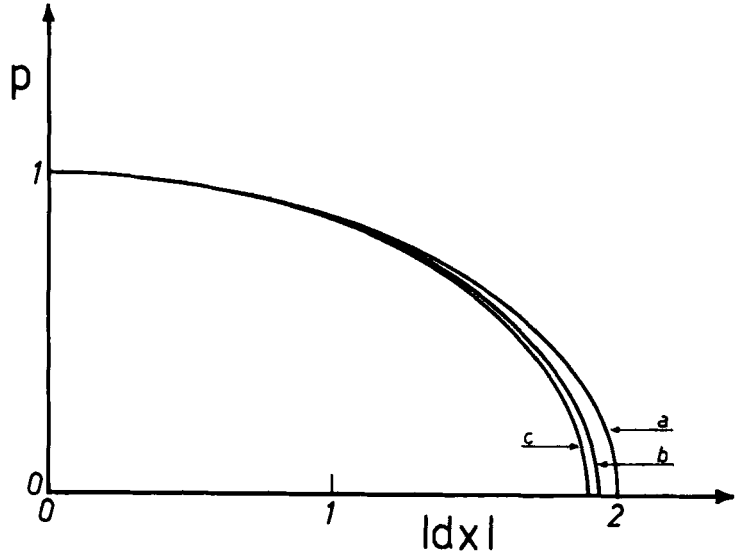

FIGURE 6 The second order polarization p vs d_x for $b_x = 0$ and (a) $z = \infty$; (b) $z = 6$; (c) $z = 4$.

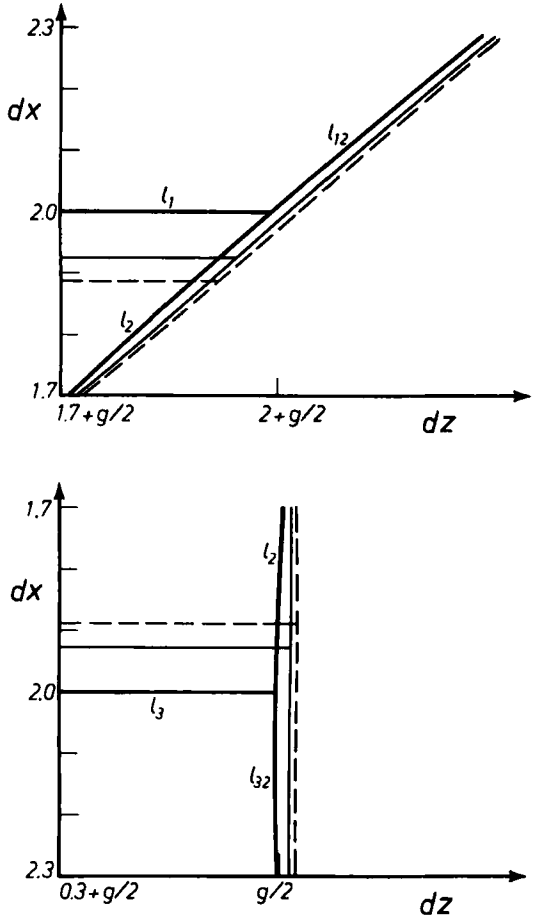

FIGURE 7 The second order phase diagram (d_z, d_x) for $b_x = 0$. The full thick line corresponds to $z = \infty$ (identical with the zero-th order). The full thin line to $z = 6$, and the broken line to $z = 4$.

corresponds to $z = \infty$). The intersection with the d_x axis defines the position of the lines l_1 ($d_x > 0$) and l_3 ($d_x < 0$). Notice that the curves in Figure 6 are independent on both g and d_z, except for the truncation the latter can induce by restricting the range of d_x, depending on the (d_z, d_x) phase diagram. The latter has a form not dissimilar from the form of Figure 1, except for the shift already noticed of lines l_1 and l_3, and the deformation of lines l_2, l_{12} and l_{32}. In proximity of $d_x = 0$ as well as asymptotically ($d_x \to \infty$) such a deformation, induced by the second order

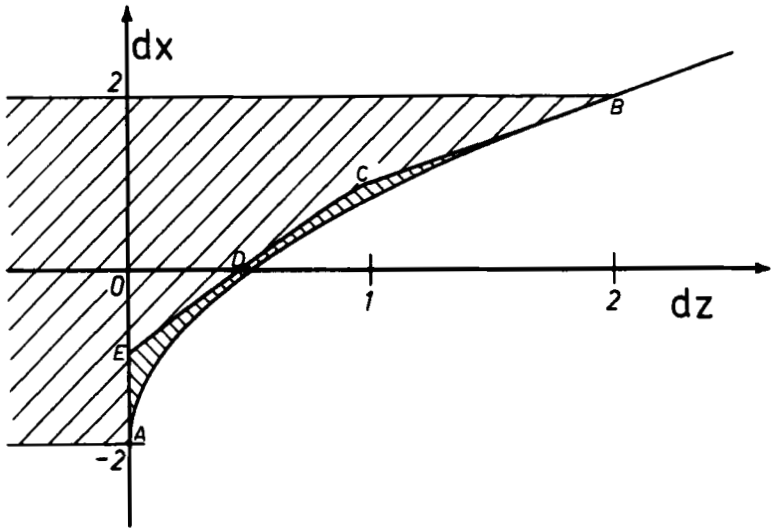

FIGURE 8 The phase plane (d_z, d_x) for $b_x = 0$ exhibiting the two zones of the ferromagnetic phase, leading to second order and first order (ABCDE) temperature dependent phase transitions (see Figure 9).

correction together with the requirement of self consistency of the theory, vanishes. The regions of the phase plane (d_z, d_x) where the effect is most noticeable are those where three phases are close to each other (F, P_1, P_2 and F, P_2, P_3 respectively). Such regions are represented in Figure 7, where the phase diagrams corresponding to $z = 4$ and $z = 6$ are compared with that of order zero.

III. Conclusions

The applications of the model described in present paper are manifold, especially from the point of view of liquid crystal physics.

The model indeed describes two types of cooperative phenomena, one of which can be interpreted — in terms of lattice-gas theory — as the usual condensation and solidification of a simple fluid.

The other one can be thought of in the following terms. If the molecules are elongated, they have a characteristic orientation, and the collective transition described by the model may then be interpreted to describe an isotropic-nematic transition of the anisotropic fluid.

Moreover, a second-order nematic transition can be found at low free energy (i.e. high pressure: in a lattice gas the pressure is but the opposite of the free energy).

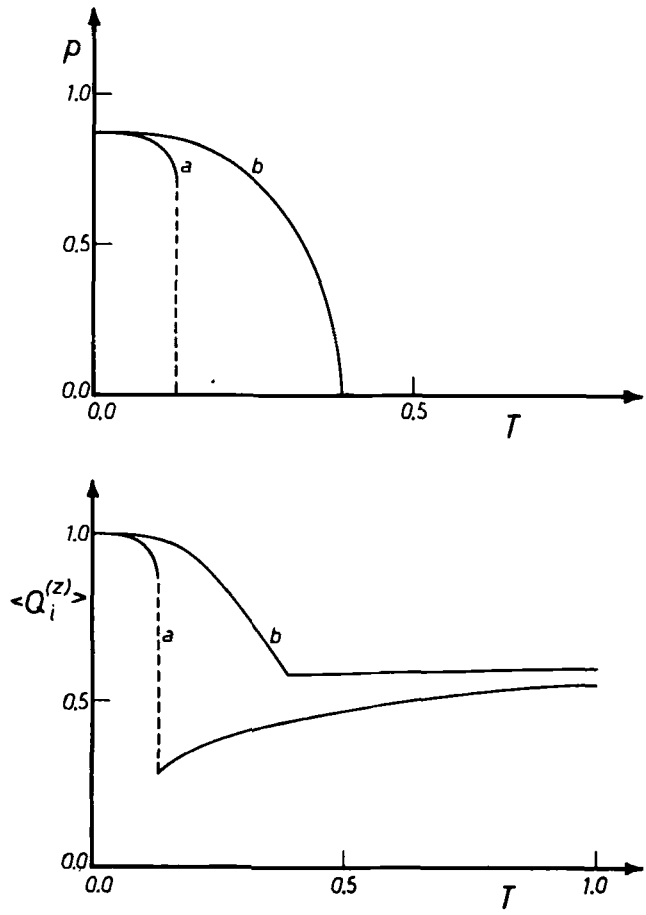

FIGURE 9 The polarization p vs temperature T for (d_r, d_z) belonging to: (a) the region (ABCDE) of Figure 8, (b) the complementary region of Figure 8.

The above interpretation is implemented by the observation that the presence of a field induces an axial symmetry, such that—in agreement with Landau's theory—for large fields the first order nematic transition disappears.

Finally it is known[10] that the isotropic-cholesteric and cholesteric-smectic-A phase transitions, namely those transitions in which crystallographic disorder is not accompanied by orientational disorder, change from the first to the second order by increasing pressure. The latter feature is exhibited by the model, as it was discussed in Section II.

To conclude, let us also mention a few preliminary results (at present limited to the simple case $b_x = 0$, $g = 0$) in which the phase diagram is enlarged to include temperature.

Using the full expression of F/N, as given by Eqs. 1.11–1.17, with β finite, the whole procedure described in Section II can be retraced. For the case under consideration, the results at order zero can be summarized by the three graphs of Figures 8 and 9. Figure 8 represents the section $T = 0$ of the 3-d phase space (d_z, d_x, T). If the couple of parameters $P \equiv (d_z, d_x)$ is hold fixed, and the temperature is increased the order parameter p and the quadrupole operator thermal average $\langle Q_i^{(z)} \rangle$ vary according to the behavior described in Figure 9.

In particular curves of type *a* corresponding to a first order phase transition are obtained when P belongs to the region ABCDE; curves of type *b* (second order transition) when P belongs to the complementary region within the ferromagnetic domain (shaded region in Figure 8).

Further work is in progress on the extension to $T \neq 0$ of the whole discussion reported in Sections I and II.

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