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SOME RESULTS OF A CLUSTER VARIATION METHOD (C.V.M.) STUDY ON THE B.C.C. LATTICE

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Abstract—Some results of cluster variation method (CVM) calculations on the BCC lattice, with an Ising hamiltonian, with first and second neighbour interactions, are presented. Apparent discrepancies, between our results and the previous ones, lead to some essential discussions. We find, (in the case $J_2/J_1 = 1$), that the transition between DO_3 and the disordered phase A2 is of second order, in contrast with previous results by other authors, who base their opinion on the Landau theory. In fact, the Landau theory establishes the possibility that this transition is of the second order type. We present this proof. An other problem appears in our CVM calculation: the presence and the stability of a new phase (always in the case $J_2/J_1 = 1$), that we call a 'four sub-lattice phase'. The surprising stability of this phase can be explained using the concept of super-degenerate point at zero temperature, between B32 and DO_3. We also present this argument. © 1997 Elsevier Science Ltd. All rights reserved

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1. INTRODUCTION

The cluster variation method (CVM) [1] has, for a long time, proved its ability and efficiency to calculate binary or ternary real phase diagrams [2–8]. It was often necessary, to do this, to make use of more complicated hamiltonians than the standard Ising one, i.e. for example the hamiltonian arising from the coherent approximation–generalized perturbation method (CPA–GPM) [9] theory.

The initial study of the CVM using a standard Ising hamiltonian has today become a basic study, interesting essentially from a fundamental point of view, but also useful for more sophisticated approaches. Whereas there have been many CVM calculations on the FCC lattice (for a review, see [9, 10]), there are only a few on the BCC one. This is a justification for the initial subject of this short paper. All the CVM calculations that we present are done on the BCC lattice, within the tetrahedron approximation, with first and second neighbour pair interactions.

We will see that some previous results already published by other authors [11–13] are not completely correct. To explain these discrepancies between our results and the previous ones, we will be leaded to some essential discussions: first around the general Landau theory and second, around the concept of super-degenerate points.

2. CVM RESULTS

We have chosen to study three basic cases corresponding to different parts of the phase diagrams at $T = 0$ (see Fig. 1):

$$J_2/J_1 = -1 \tag{1}$$

$$J_2/J_1 = 0.5 \tag{2}$$

$$J_2/J_1 = 1 \tag{3}$$

Our results relative to the equations (1)–(3) are presented respectively in Figs 2–4a. We reproduce also the results obtained previously by other authors, in Fig. 5 for the case of equation (1) (see Ref. [11]), in Fig. 6 for the case of equation (2) (see Refs [11, 13, 14]), in Fig. 7 for the case of equation (3) (see Refs [11–13]) (the results are symmetrical with regard to the concentration 0.5).

For the case of equation (1), our result in Fig. 2a and b is in perfect agreement with the result already published in Fig. 5 (Ref. [11]), and needs to comment. For the case of equation (2), we find the same diagram as in most results previously published (see Fig. 6b and c, and Refs [13, 14]). Golosov and Tolstik (Ref. [11], Fig. 6a) do not find that a part of the DO_3–B2 transition is of the first order. If a very attentive calculation is made, we see that it is only the point of numerical precision. For the case of equation (3), we find many differences between our results and the previous ones. We find, first, that the transition between the ordered phase DO_3 and the disordered one A2, is of the second order type, in agreement with Golosov and Tolstik (Ref. [11], Fig. 7a), Inden (Ref. [13], Fig. 7b), and in contrast with Sluiter and Turchi (Ref. [12], Fig. 7c). According to Sluiter and Turchi, the Landau theory implies inevitably that the transition DO_3–A2 is of the first order type.

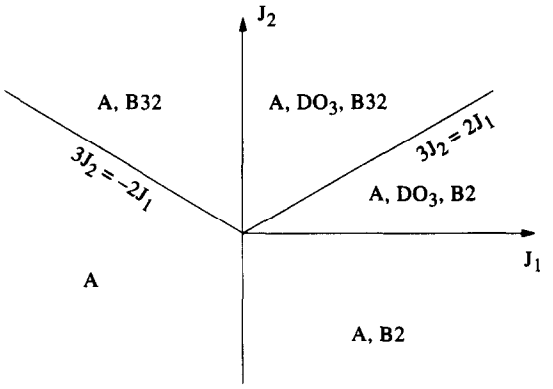

Fig. 1. Phase diagram on the BCC lattice $T=0$. J_1, J_2 are the first and second neighbour interactions.

Another important difference, this time with all the previously published results (see Refs [11–13]), is the presence of a new phase in our CVM calculation (see Fig. 4), that we call the 'four sub-lattice phase' (for all phases, see Fig. 8), between DO_3 and B32 (Golosov and Tolstik [11] found a two-phase regime between B32 and DO3, Sluiter and Turchi [12] also found a two-phase regime, and Inden [13] found a second order transition between DO_3 and $F\bar{4}3m$, and between $F\bar{4}3m$ and B32). We must discuss now in the next paragraphs both of these apparent discrepancies in some detail.

3. STUDY OF THE ORDER OF THE TRANSITION DO_3–A2

We present here a general argument, based on the Landau theory.

Let F be the free energy function: $F(\{c_n\})$ (function of the concentration c_n in site n). Let us consider that c_n is slightly different from the average concentration, $c_n = c + \delta c_n$. We proceed now to a wave concentration expansion:

$$F(\{c_n\}) = F(c) + \sum_n \delta c_n F_n^{(1)} + \sum_{nm} \delta c_n \delta c_m F_{nm}^{(2)} + \sum_{nmp} \delta c_n \delta c_m \delta c_p F_{nmp}^{(3)} + \sum_{nmpq} \delta c_n \delta c_m \delta c_p \delta c_q F_{nmpq}^{(4)} + \cdots$$

with $F_n^{(1)} = \dfrac{\delta F(c)}{\delta c_n}$, etc...we have: $\sum_n c_n = 0$ (because $\sum_n c_n = c$).

A Fourier transformation of the last expression gives:

$$\delta F = \sum_{\mathbf{k}} I \delta c_{\mathbf{k}} I^2 F^{(2)}(\mathbf{k}) + \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''} \delta c_{\mathbf{k}} \delta c_{\mathbf{k}'} \delta c_{\mathbf{k}''} \delta(\mathbf{k}+\mathbf{k}'+\mathbf{k}''-\mathbf{K}) F^{(3)}(\mathbf{k},\mathbf{k}',\mathbf{k}'') + \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta c_k, \delta C_{\mathbf{k}'} \delta c_{\mathbf{k}''} \delta c_{\mathbf{k}'''} \delta(\mathbf{k}+\mathbf{k}'+\mathbf{k}''+\mathbf{k}'''-\mathbf{K}) \times F^{(4)}(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''') + \cdots$$

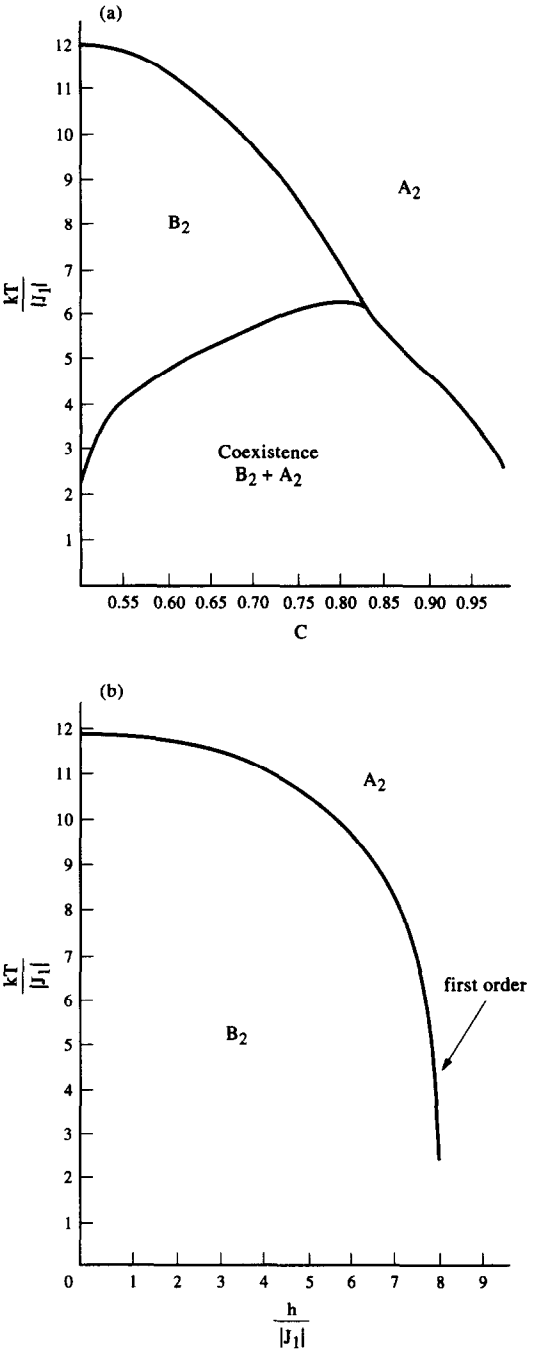

Fig. 2. Phase diagrams calculated, with $J_1 > 0, J_2/J_1 = -1$, with respect to the field (a), and to the concentration (b).

(**K** is a vector of the reciprocal lattice).

If we limit this summation to the **k**-vectors associated to DO_3: $\mathbf{k}_1 = \langle 100 \rangle$ and $\mathbf{k}_2 = \langle 111/222 \rangle$, the expansion becomes:

$$F = a\eta^2 + b\gamma^2 + c\eta^2\gamma + d\eta^4 + e\gamma^4 + \cdots$$