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Diffusion coefficients of fluctuations in semi-infinite ferromagnets

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Résumé. — Nous appliquons le modèle d'Ising avec interactions entre proches voisins au cas d'un ferromagnétique semi-infini, les interactions en surface pouvant être différentes de celles en volume. Les fluctuations d'aimantation au voisinage de transitions du deuxième ordre sont décrites par une équation de diffusion contenant un terme d'amortissement. Le coefficient de diffusion des fluctuations paramagnétiques est obtenu en champ moyen pour les transitions en volume, en surface-volume et en surface et nous discutons leur variation avec la distance à la surface et la température.

Abstract. — The nearest-neighbour Ising model of a semi-infinite ferromagnet in which near-surface couplings may differ from their bulk values is considered. In the critical region near second-order phase transitions the decay of fluctuations of the magnetization density is described by a diffusion equation with a damping term. Using mean-field theory, the diffusion coefficients of fluctuations in the paramagnetic phase near the ordinary, surface-bulk and surface phase transitions are obtained and their dependence on the distance from the surface of the ferromagnet and on the temperature is discussed.

We consider the nearest-neighbour simple cubic Ising model of a semi-infinite ferromagnet. The coordinates of a lattice site are denoted by (ij) where i denotes the number of the two-dimensional layer parallel to a surface of the ferromagnet whereas j is a two-dimensional vector within each layer. We denote by $K_{ii'}$ the nearest-neighbour exchange interaction between spins in layers i and i' divided by the Boltzmann constant and the temperature. It equals $K(1 + D)$ when both nearest neighbours are situated in a surface layer and K for all other nearest-neighbour pairs. In the critical region near a continuous phase transition the decay of fluctuations of the magnetization density $\bar{m}_{ij}(t)$ at a position (ij) is described by a diffusion equation with a damping term. In the paramagnetic phase this equation can be written in the following form [1]

$$\frac{\partial \bar{m}_{ij}(t)}{\partial t} = \frac{1}{T_i} \left(-\bar{m}_{ij}(t) + \frac{1}{2} \sum_{i'j'} K_{ii'} \bar{m}_{i'j'}(t) \right) \quad (1)$$

where the summation runs over the nearest neighbours of a position (ij) and T_i denotes the spin lattice relaxation time in the i -th layer. The model of a semi-infinite ferromagnet has been

studied using mean-field theory [2-4], the renormalization-group approach [5-7] and numerical techniques [3]. In this paper we apply mean-field theory to obtain the diffusion coefficients of fluctuations in the paramagnetic phase near the ordinary, surface-bulk and surface phase transitions. In mean-field theory the diffusion coefficients depend on the distance from the surface of the semi-infinite ferromagnet and on the temperature. Mean-field theory often produces a correct qualitative picture and using this theory almost all quantities of interest can be calculated analytically.

We denote by A_i the diffusion coefficient of the fluctuations in the i -th layer. It describes a diffusion of the magnetization density in the layer. We apply to A_i the self-consistent procedure proposed by Kawasaki [8, 9] for the diffusion coefficient of fluctuations in an infinite three-dimensional ferromagnet in the paramagnetic phase. We obtain, as in [10], that A_i is proportional to $(L_i/\chi_i)^{1/2}$ where L_i denotes the autocorrelation time in the i -th layer divided by T_i whereas χ_i is the magnetic susceptibility in the i -th layer. In order to obtain L_i , let us consider the Ising model of ferromagnetic film with both surfaces the same as the surface of the considered semi-infinite ferromagnet. Following the procedure described in [1] and finding the limit of obtained formulae for the thickness of the film tending to infinity we obtain

$$L_i = \frac{1}{\text{sh } x} + \frac{e^{-2ix}}{(1 - 4D e^{-x})} \left(\frac{4D e^x - 1}{\text{sh } x} - \frac{e^{2x} - 1}{\text{sh } x + 2} \right) \quad (2)$$

where x is determined by the following equation

$$\text{ch } x = K^{-1} - 2. \quad (3)$$

The magnetic susceptibility χ_i in the semi-infinite ferromagnet, defined as a derivative of the magnetization in the i -th layer with respect to the external uniform magnetic field, can be written in the form [4]

$$\chi_i \sim \frac{1}{\text{sh}^2\left(\frac{x}{2}\right)} \left(1 + \frac{4D - 1}{(1 - 4D e^{-x})} e^{-ix} \right). \quad (4)$$

The magnetic susceptibility χ_i tends to infinity for x tending to zero which determines the ordinary phase transition line and the surface-bulk phase transition point or for $(1 - 4D e^{-x})$ tending to zero which determines the surface phase transition line. We denote by T_c the temperature of a phase transition and by ϵ the reduced temperature defined as $T/T_c - 1$.

The diffusion coefficient of fluctuations A_i depends on two quantities L_i and χ_i which have different critical behaviours. The magnetic susceptibility χ_i depends on all correlations in a system [4] whereas L_i depends only on correlations in the i -th layer [1] so, in any layer of the semi-infinite ferromagnet, the critical behaviour of χ_i begins at temperatures farther from T_c than the critical behaviour of L_i . The critical behaviour of A_i at temperatures farther from T_c is thus determined by the critical behaviour of χ_i whereas at temperatures very near T_c it is mainly determined by the critical behaviour of L_i .

The diffusion coefficients in layers near the surface of semi-infinite ferromagnets with different values of D are shown in figure 1. According to the value of D , curves in this figure show the behaviour of the diffusion coefficients near the ordinary ($D < 1/4$), the surface-bulk ($D = 1/4$) or the surface ($D > 1/4$) phase transition. In the critical region near any phase transition the diffusion coefficients of fluctuations decrease when the temperature tends to T_c . The ordinary phase transition is induced by all interactions in the ferromagnet whereas the surface phase transition is induced only by large surface interactions so the diffusion coefficients of fluctuations near the ordinary and the surface phase transitions behave differently. At temperatures near

Fig. 1. — The diffusion coefficients of fluctuations A_i in layers near the surface of semi-infinite ferromagnets with different values of D for reduced temperatures 2^{-7} (a), 2^{-9} (b), 2^{-11} (c), 2^{-13} (d), 2^{-15} (e) and 2^{-17} (f).

the ordinary phase transition, the diffusion coefficients in different layers far from the surface of the semi-infinite ferromagnet are equal and do not depend on D . They slightly increase in layers near the surface over a distance which approximately equals the average correlation length. At temperatures near the surface phase transition, the diffusion coefficients in layers far from the surface of the ferromagnet are determined by the extraordinary phase transition. In layers near the surface, correlations of a spin with spins on the surface dominate and they determine the critical behaviour of physical quantities. The critical behaviour of χ_i induced by large surface interactions begins in layers farther from the surface of the ferromagnet than the critical behaviour of L_i because χ_i contains correlations with the surface, whereas L_i contains only correlations within the layer. Therefore, at temperatures near the surface phase transition temperature, when we approach the surface of the ferromagnet, A_i first decreases because χ_i quickly increases whereas very near the surface A_i increases because L_i quickly increases. In layers farther from the surface of the semi-infinite ferromagnet where the diffusion coefficients of fluctuations decrease, all correlations determine the critical behaviour of physical quantities. In layers near the surface where the diffusion coefficients increase, the nearest correlations dominate and determine the critical behaviour of physical quantities.

In systems with surfaces it is necessary to define a certain number of new critical exponents which refer to local physical quantities [3]. We define the critical exponent $w(A_i)$ of the diffusion coefficient of fluctuations A_i as the derivative of $\ln A_i$ with respect to $\ln \epsilon$. Critical exponents $w(A_i)$ in the range of reduced temperatures between 2^{-7} and 2^{-15} in some layers of semi-infinite ferromagnets with different values of D are shown in figure 2. When ϵ decreases, the critical exponent $w(A_i)$ in any layer farther from the surface of the semi-infinite ferromagnet changes from the value like that in an infinite three-dimensional ferromagnet to the value like that in the surface layer. At temperatures farther from T_c the exponent $w(A_i)$ changes like $w(\chi_i)$ because $w(L_i)$ is constant whereas at temperatures near T_c it changes like $w(L_i)$ because $w(\chi_i)$ is already constant. In the semi-infinite ferromagnet with D equal to zero, the critical exponent $w(A_i)$ equals 0.25 at temperatures very far and very near T_c . In a certain range of temperatures it however tends to another value because $w(\chi_i)$ and $w(L_i)$ change in different ranges of temperatures. In the semi-infinite ferromagnet with a great value of D , the exponent $w(A_i)$ at temperatures far from the surface phase transition temperature T_c equals zero and it increases at temperatures where χ_i dominates. At temperatures very near T_c , the quantity L_i increases and $w(A_i)$ in any layer tends to the value $w(A_1)$ as in the surface layer. The value of $w(A_1)$ is in this case the same as in an infinite two-dimensional ferromagnet.

In the semi-infinite ferromagnet with D between 0.25 and 0.4, the distance between the temperatures of the surface and the extraordinary phase transitions is small so the extraordinary phase transition has an effect on the behaviour of critical exponents near the surface phase transition. In such a ferromagnet, the critical exponent $w(A_i)$ in any layer at temperatures farther from the surface phase transition temperature is determined by the extraordinary phase transition and when ϵ decreases the exponent calculated with respect to the surface phase transition temperature tends to zero. At temperatures very near the surface phase transition temperature, the term $1/(1 - 4D\epsilon^{-x})$ (formulae 2 and 4) is the most important so $w(A_i)$ behaves as described above in the semi-infinite ferromagnet with a great value of D . In the mean-field theory the critical exponent $w(\chi_i)$ equals -1 in an infinite two- and three-dimensional ferromagnet. In the semi-infinite ferromagnet with D equals to 0.25 the changes of $w(A_i)$ in any layer near the surface-bulk phase transition are thus caused by the changes of the exponent $w(L_i)$. Comparing dependences of $w(A_i)$ on the reduced temperature in the same layers of semi-infinite ferromagnets with D equals to 0 and 0.25, it is seen that $w(L_i)$ and $w(\chi_i)$ change in different ranges of temperatures.

We conclude that in the critical region near a second-order phase transition, a physical quantity which consists of some other quantities in a certain range of temperatures has the same

Fig. 2. — Critical exponents of the diffusion coefficients of fluctuations $w(A_i)$ in some layers of semi-infinite ferromagnets with different values of D in the range of reduced temperatures between 2^{-7} and 2^{-15} . The reduced temperature is 2^{-l} where l is on the horizontal axis.

critical exponent behaviour and satisfies the same scaling relations as does its component quantity whose critical behaviour dominates in this range. In any position of a semi-infinite system at temperatures far from the temperature of a continuous phase transition, the critical behaviours of physical quantities are determined by the phase transition induced by internal interactions in the system. Critical exponents of physical quantities are in this case like those in an infinite three-dimensional system. At temperatures very near a phase transition temperature, the critical behaviours of physical quantities are determined by two-dimensional phase transition induced only by large surface interactions or they are determined by the phase transition induced by both surface and internal interactions. In this case critical exponents of physical quantities in any position of a semi-infinite system are the same as on the surface of the system.

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