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CRITICAL BEHAVIOUR OF THE SEMIINFINITE TRANSVERSE ISING MODEL

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Юлия Веселинова. КРИТИЧНО ПОВЕДЕНИЕ НА ПОЛУБЕЗКРАЕН НАПРЕЧЕН МОДЕЛ НА ИЗИНГ

Като се използва методът на функциите на Грин е разгледан тримерният напречен модел на Изинг с модифицирано обменно взаимодействие на повърхността. Полученият критичен показател за възприемчивостта на повърхностния слой е $\gamma_s = 1{,}81 \pm 0{,}012$ за кубична решетка и $\gamma_s = 2{,}10 \pm 0{,}012$ за квадратична решетка (който е различен в сравнение с обема $\gamma = 1{,}229 \pm 0{,}012$ за кубична решетка). Това съвпада с резултатите от методите на ренорм-групата и Монте Карло.

Julia Wesselinowa. CRITICAL BEHAVIOUR OF THE SEMIINFINITE TRANSVERSE ISING MODEL

Usung a Green's function technique we have investigated a three-dimensional Ising model with modified surface exchange. The surface layer-susceptibility exponent is obtained as $\gamma_s = 1.81 \pm 0.012$ for a cubic lattice and $\gamma_s = 2.10 \pm 0.012$ for a square lattice (which is different compared with the bulk $\gamma = 1.229 \pm 0.012$ for a cubic lattice) and is in agreement with results using the renorm-group and the Monte Carlo methods.

Keywords: critical exponent, surface layer-susceptibility, semiinfinite transverse Ising model, Green's function technique

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INTRODUCTION

Theoretical treatments of phase transitions usually consider ideal crystals of infinity extent. Experiments, however, are carried out on samples of finite size: there may be a need to consider the effects of both external surfaces of the system and internal ones such as grain boundaries and other kinds of interface. The critical behaviour at surfaces [1] is complicated by the fact that, apart from the geometrical effect of "missing neighbours", the microscopic interactions close to the surface may have values which are quite different from those deep in the bulk. As a result, the surface may order bevore the bulk, or may even exhibit ordering phenomena of a different character than the bulk, such as an antiferromagnetic transition at the surface of a ferromagnetic material, etc. Thus surfaces may constitute interesting examples of low-dimensional orderings. While there is as yet no experimental evidence that this type of truly two-dimensional order actually occurs in magnet, there is a wealth of experimental evidence for structural phase transitions at surfaces ("surface reconstruction").

Just as the critical behaviour of the bulk free energy can be described in terms of critical exponents and scaling concepts, a similar description emerges for the surface free energy, too. For example, the divergence of the surface specific heat at the critical point is then described by the "surface exponent" α_s, which differs from the exponent α_b describing the divergence of the specific heat in the bulk. The surface susceptibility χs was first studied by Allen [2] who concluded that $\gamma_{\mathrm{s}} = 1.95 \pm 0.08$. The series for χ_{s} was then extended by Capehart and Fisher [3]. More extensive works exist on the $n \to 0$ limit of the n-vector model, which is physically applicable to the problem of polymer statistics near walls. A direct estimate of γ_{s} from walks up to 21 steps [4] yields $\gamma_{\mathrm{s}} = 2.10 \pm 0.01$. Using walks up to 14 steps Whittington et al. [4] found $\gamma_{\mathrm{s}} = 1.81 \pm 0.02$ for $d = 3$. Landau [5] studied the surface specific heat C_s and surface susceptibility χ_{s} both for square and simple cubic Ising system with nearest neighbour interaction. In this work on systems with finite linear dimensions in all directions, the Monte Carlo results were found to be consistent with the finite size scaling description. Landau finds $\gamma_{\mathrm{s}} = 1.8 \pm 0.02$ for $d = 3$. From measurements of the temperature dependence of the static susceptibility for a Gd monolayer Farle and Baberschke [6] obtained $\gamma \approx 1.8$.

The Ising model in a transverse field (TIM) is widely employed to describe the critical behaviour of the order-disorder transitions in H-bonded ferroelectrics, for an excellent review on recent activities and in the past, see Ref. [7]. The critical exponent of the central peak and the soft-mode peak widths Δ_c and Δ_{s} are calculated in Refs. [8–11]. Similarly to the critical dynamics of classical spin models at finite temperatures one can expect that the critical exponents of the quantum models are also universal.

THE MODEL AND THE MATRIX GREEN'S FUNCTION

The aim of the present paper is to calculate the critical exponent γ_{s} for the surface layer-susceptibility of H-bonded ferroelectrics based on the TIM using a Green's function technique beyond the RPA for semiinfinite TIM, the Hamiltonian of which is written as:

$$H = -\frac{1}{2}\sum_{ij} J_{ij} S_i^z S_j^z - \Omega_{\mathrm{b}} \sum_{i\in \mathrm{b}} S_i^x - \Omega_{\mathrm{s}} \sum_{i\in S} S_i^x - \mu E \sum_i S_i^z , \qquad (1)$$

where S^x and S^z are components of spin-1/2 operators, and Ω_{b} and Ω_{s} represent transverse fields in the bulk and surface layers, and the sums are over the internal and surface lattice points, respectively. J_{ij} is an exchange interaction between spins at nearest-neighbour sites i and j, and $J_{ij} = J_{\rm s}$ between spins on the surface layer, otherwise it is $J_{\rm b}$. E is an external electrical field in z-direction. In the ordered phase we have the mean values $\langle S^x \rangle \neq 0$ and $\langle S^z \rangle \neq 0$, and it is appropriate to choose a new coordinate system rotating the original one used in (1) by the angle θ in the xy plane [12]. The rotation angle θ is determined by the requirement $\langle S^x \rangle = 0$ in the new coordinate system.

The retarded Green's function to be calculated is defined as

$$G_{ij}(t) = \langle\langle b_i(t); b_j^+(0) \rangle\rangle, \tag{2}$$

where b and b^+ are the Pauli operators in the rotated system. On introducing the two-dimensional Fourier transform $G_{n_i n_j}(\vec{k}_\|, \omega)$, one has the following form:

$$\langle\langle b_i; b_j^+ \rangle\rangle_\omega = \frac{\sigma}{N'} \sum_{\vec{k}_{||}} \exp(i\vec{k}_{||}(\vec{r}_i - \vec{r}_j)) G_{n_i n_j}(\vec{k}_{||}, \omega), \tag{3}$$

where N' is the number of sites in any of the lattice planes, $\vec{r}_i$ and n_i represent theposition vectors of site i and the layer index, respectively, $\vec{k}_\|$ is a two-dimensional wave vector parallel to the surface. The summation is taken over the Brillouin zone.

As a result the equation of motion for the Green's function (3) of the semi-infinite ferroelectrics for $T \leq T_C$ has the following matrix form:

$$H(\omega) G(\vec{k}_{||}, \omega) = R, \tag{4}$$

where H, G and R are $\infty \times \infty$ matrices. H can be expressed as:

$$H = \begin{pmatrix} \omega - V & k_1 & 0 & 0 & 0 & 0 & \dots \\ k & \omega - U & k & 0 & 0 & 0 & \dots \\ 0 & k & \omega - Q & k & 0 & 0 & \dots \\ 0 & 0 & k & \omega - Q & k & 0 & \dots \\ . & . & . & . & . & . & \dots \end{pmatrix}_{\infty \times \infty}$$

with

$$\begin{aligned} k_1 &= J_{\rm b} \sigma_{\rm s} \sin^2 \theta_{\rm s}, \qquad\qquad k = J_{\rm b} \sigma_{\rm b} \sin^2 \theta_{\rm b}, \\ V &= \varepsilon_{\rm s} + \frac{1}{N\sigma_{\rm s}} \sum_{\vec{q}} \Bigg(\frac{\sin^2 \theta_{\rm s}}{2} J_{\rm s}(\vec{q}) \langle b_{\vec{q}}^+; b_{-\vec{q}}^+ \rangle_{\rm s} - V_{\rm s}(\vec{k}_\| - \vec{q}, \vec{q}) \langle b_{\vec{q}}^+; b_{\vec{q}} \rangle_{\rm s} \\ &\quad + J_{\rm b} \sigma_{\rm b} \sigma_{\rm s} \cos^2 \theta_{\rm b} + \mu E \cos \theta_{\rm s} \Bigg), \\ U &= \varepsilon_{\rm b} + \frac{1}{N\sigma_{\rm b}} \sum_{\vec{q}} \Bigg(\frac{\sin^2 \theta_{\rm b}}{2} J_{\rm b}(\vec{q}) \langle b_{\vec{q}}^+; b_{-\vec{q}}^+ \rangle_{\rm b} - V_{\rm b}(\vec{k}_\| - \vec{q}, \vec{q}) \langle b_{\vec{q}}^+; b_{\vec{q}} \rangle_{\rm b} \end{aligned}$$

$$
\begin{aligned}
& +J_{\mathrm{s}}\sigma_{\mathrm{s}}\sigma_{\mathrm{b}}\cos^2\theta_{\mathrm{s}} + J_{\mathrm{b}}\sigma_{\mathrm{b}}^2\cos^2\theta_{\mathrm{b}} + \mu E\cos\theta_{\mathrm{b}}\Bigg), \\
Q &= \varepsilon_{\mathrm{b}} + \frac{1}{N\sigma_{\mathrm{b}}}\sum_{\vec{q}}\Bigg(\frac{\sin^2\theta_{\mathrm{b}}}{2}J_{\mathrm{b}}(\vec{q})\langle b_{\vec{q}}^{+}; b_{-\vec{q}}^{+}\rangle_{\mathrm{b}} - V_{\mathrm{b}}(\vec{k}_{\|}-\vec{q},\vec{q})\langle b_{\vec{q}}^{+}; b_{\vec{q}}\rangle_{\mathrm{b}} \\
& +J_{\mathrm{b}}\sigma_{\mathrm{b}}^2\cos^2\theta_{\mathrm{b}} + \mu E\cos\theta_{\mathrm{b}}\Bigg), \\
J(\vec{k}_{\|}) &= \frac{J}{2}(\cos(k_x a) + \cos(k_y a)), \\
\varepsilon &= 2\Omega\sin\theta + \frac{\sigma}{2}J\cos^2\theta - \frac{\sigma}{4}J(\vec{k}_{\|})\sin^2\theta, \\
V(\vec{q},\vec{k}_{\|}-\vec{q}) &= J(\vec{q})\cos^2\theta - \frac{1}{2}J(\vec{k}_{\|}-\vec{q})\sin^2\theta.
\end{aligned}
$$

$\sigma(T)$ is the relative polarization in the direction of the mean field and is equal to $2\langle S^{z'}\rangle$. The correlation functions are calculated from the Green's functions using the Spectral theorem. For the rotation angle θ we have the following two solution in the generalized Hartree-Fock approximation:

1. $\cos\theta = 0$, i.e. $\theta = \frac{\pi}{2}$, if $T \geq T_C$;
2. $\sin\theta = \frac{4\Omega}{\sigma J} = \frac{\sigma_c}{\sigma}$, if $T \leq T_C$.

In order to obtain the solutions of the matrix equation (4), we define two-dimensional column matrices, G_n and R_n with the elements given by $(G_n)_m = G_{nm}$ and $(R_n)_m = \sigma_n\delta_{mn}$, so that equation (4) yields:

$$H(\omega)G_n = R_n \ , \tag{5}$$

which could be resolved easily by reference to the transfer-matrix method [13, 14]. We introduce the two transfer functions:

$$T_1 = \frac{G_{2i+1,m}}{G_{2i,m}}, \quad T_2 = \frac{G_{2i,m}}{G_{2i-1,m}} \quad (i \geq 1). \tag{6}$$

Substituting T_1 and T_2 into one column of (5), the following Green's functions can be obtained:

$$
\begin{aligned}
G_{11} &= \frac{1}{\omega - V + k_1 T_2}, && (7) \\
G_{22} &= \frac{1}{\omega - U + \left(kT_1 - \dfrac{k_1 k}{\omega - V}\right)}, && (8)
\end{aligned}
$$

$$G_{33} = \frac{1}{\omega - Q + \left(kT_2 - \cfrac{k^2}{\omega - U - \cfrac{k_1 k}{\omega - U - \cfrac{k_1 k}{\omega - V}}} \right)}, \tag{9}$$

and so on, where

$$T_1 = \frac{1}{2k}\left(-\omega + U \pm \sqrt{\omega - U - 4k^2 \frac{\omega - U}{\omega - Q}}\right), \tag{10}$$

$$T_2 = \frac{1}{2k}\left(-\omega + Q \pm \sqrt{\omega - Q - 4k^2 \frac{\omega - Q}{\omega - U}}\right). \tag{11}$$

As it is well known, the poles of the Green's functions give the dispersion relation of the spin waves, therefore the surface spin wave (SSW) spectrum can be given from Eq. (7) by the following expression:

$$\omega_{\mathrm{s}} - V(\omega_{\mathrm{s}}) + k_1 T_2(\omega_{\mathrm{s}}) = 0, \tag{12}$$

which has to be numerically calculated.

The so obtained SSW's can be used for the evaluation of the relative polarization of the surface σ_{s}:

$$\sigma_{\mathrm{s}} = \left(\frac{\sigma_{\mathrm{s}}}{2N} \sum_{\vec{k}_{\parallel}} \frac{J_{\mathrm{s}} - 0.5\sin^2\theta_{\mathrm{s}} J_{\mathrm{s}}(\vec{k}_{\parallel})}{\omega_{\mathrm{s}}} \coth\frac{\omega_{\mathrm{s}}}{2T} \right)^{-1}. \tag{13}$$

However, the surface polarization involves the SSW's, the bulk polarization and the bulk energy, so that all expressions must be solved self-consistently.

THE CRITICAL EXPONENT OF THE SURFACE SUSCEPTIBILITY

The longitudinal susceptibility χ^{zz} in the ordered phase is determined by the relation $\mathrm{d}\langle S^z\rangle / \,\mathrm{d}E|_{E=0}$. Taking into account that for small field E

$$\cos\theta \approx 0.5 \frac{\mu E}{\Omega - \sigma J_0/4}, \tag{14}$$

we obtain for χ_{s}^{zz}:

$$\chi_{\mathrm{s}}^{zz}(E=0) = \frac{0.5\sigma_{\mathrm{s}}}{\Omega_{\mathrm{s}} - \sigma_{\mathrm{s}} J_{\mathrm{s}}/4}. \tag{15}$$

The temperature dependence of $\sigma_{\rm s}$ and of $\chi_{\rm s}^{zz}$ was calculated numerically using parameters appropriate to the H-bonded ferroelectric KDP [15]: $J_{\rm b} = 495$ K, $\Omega_{\rm b} = 124$ K. The critical exponent $\gamma_{\rm s}$ for the longitudinal susceptibility $\chi_{\rm s}^{zz}$ is determined for a three-dimensional cubic lattice and for a square lattice for $J_{\rm s} = 0.2J_{\rm b}$ and $\Omega_{\rm s} = 0.2\Omega_{\rm b}$ in the temperature range $5\times10^{-4} < |T_C - T/T_C| < 5\times10^{-3}$. We obtaine the following values:

$$\gamma_{\rm s} = 1.81 \pm 0.012; \quad 2.10 \pm 0.012 \tag{16}$$

for a simple cubic lattice and for a square lattice, respectively. Notice, that the value of γ for a bulk material is $\gamma = 1.229 \pm 0.012$ [12]. The obtained results (16) are in agreement with the theoretical results of Whittington et al. [4], Le Guillou and Zinn-Justin [16] and the experimental data of Farle and Baberschke [6].

In conclusions, using for the first time a Green's function formalism beyond the RPA, the critical exponent γ_s for the surface-layer susceptibility $\chi_{\rm s}^{zz}$ is calculated for a semiinfinite transverse Ising model. We obtain for a cubic lattice $\gamma_{\rm s} = 1.81 \pm 0.012$ and for a square lattice $\gamma_{\rm s} = 2.10 \pm 0.012$ in agreement with the experimental data and with the theoretical results from the renorm-group and the Monte Carlo methods.

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