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Surface critical behaviour near the uniaxial Lifshitz point of the axial next-nearest-neighbour Ising model

H L Frisch†, J C Kimball‡ and Kurt Binder§

† Department of Chemistry, The State University of New York at Albany, 1400 Washington Avenue, Albany, NY 12222, USA

‡ Department of Physics, The State University of New York at Albany, 1400 Washington Avenue, Albany, NY 12222, USA

§ Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Staudinger Weg 7, Germany

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Abstract. The semi-infinite axial next-nearest-neighbour Ising (ANNNI) model in the disordered phase is treated within a molecular-field approximation, and the singularities of various response functions characterizing the critical behaviour at the surface are obtained. In previous work (Binder K and Frisch H L 1999 *Eur. Phys. J.* B **10** 71) the axis where a nearest-neighbour ferromagnetic (J_1) and next-nearest-neighbour antiferromagnetic (J_2) exchange compete was chosen perpendicular to the surface plane. In the present work we consider an orientation of this axis parallel to the surface, allowing also for different values of these exchange interactions (j_1, j_2) in the surface plane. We derive the conditions for the occurrence of a surface transition, where the surface plane (at a temperature where the bulk is still disordered) orders either ferromagnetically or into a modulated structure. At the ordinary transition of the surface we obtain the mean-field values of the surface critical exponents, including the Lifshitz point of the bulk, where $\gamma_1^L = 1/2$, $\gamma_{11}^L = -1/2$, $\eta_\perp^L = 0$, $\eta_\parallel^L = 3$. These exponents differ from their counterparts for the case where the axis of competing interactions is oriented perpendicular to the surface, and thus it is shown that for a uniaxial Lifshitz point the surface critical behaviour depends on the surface orientation.

1. Introduction

The axial next-nearest-neighbour Ising (ANNNI) model [1–5] is an archetypical model describing how competing interactions in a solid can give rise to incommensurately modulated order and uniaxial Lifshitz points [4–7]. In this model, sites i of a (hyper-) cubic d-dimensional lattice carry Ising spins $S_i = \pm 1$, which interact in $d - 1$ directions with a nearest-neighbour ferromagnetic exchange interaction J_0, while in the remaining direction (z) there is a competition between a nearest-neighbour ferromagnetic exchange $J_1 > 0$ and a next-nearest-neighbour antiferromagnetic exchange $J_2 < 0$. If the ratio $\kappa = -J_2/J_1$ exceeds a particular value κ_L ($\kappa_L = 1/4$ in molecular-field theory [4, 5]), the system undergoes a (second-order) phase transition at a temperature $T_{mb}(\kappa)$ from the disordered phase to a phase whose order is modulated in the z-direction with a wavelength $\lambda = 2\pi/q(\kappa)$ with $q(\kappa) \propto (\kappa - \kappa_L)^{\beta_q}$ [6, 7], the exponent β_q in mean-field theory being $\beta_q = 1/2$. At the Lifshitz point ($\kappa = \kappa_L$, $T = T_L = T_{cb}(\kappa = \kappa_L) = T_{mb}(\kappa = \kappa_L)$; see figure 1 for a partial phase diagram of the ANNNI model in the molecular-field approximation) there is no longer any modulation, but the critical behaviour is anisotropic since the wavevector-dependent susceptibility $\chi(\vec{q}_\parallel, q_z)$

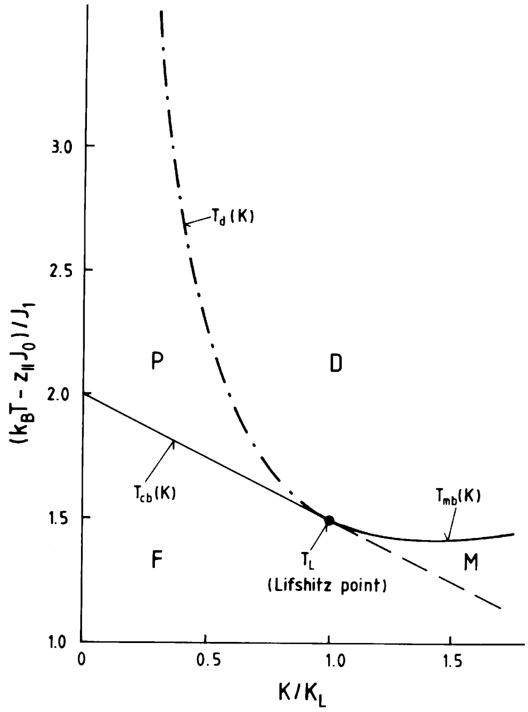

Figure 1. The phase diagram of the ANNNI model for the bulk in the molecular-field approximation, in the plane of variables $(k_BT - z_{\parallel}J_0)/J_1$ and $\kappa = -J_2/J_1$, $z_{\parallel}$ being the coordination number in the (hyper-) plane normal to the z-direction. The phase transition occurs from a paramagnetic phase (P), characterized by a monotonically decaying correlation function, to a ferromagnetic phase (F) at $T = T_{cb}(\kappa)$ for $\kappa \leqslant \kappa_L$, with $k_BT_{cb}(\kappa) = z_{\parallel}J_0 + 2J_1(1-\kappa)$. The end point of this line, $T_L = T_{cb}(\kappa = \kappa_L)$, is the Lifshitz point. For $\kappa > \kappa_L$ one has a transition from a disordered phase (D), where the correlation function exhibits an oscillatory decay, to a phase with modulated periodic order at $T = T_{mb}(\kappa) = T_{cb}(\kappa) + J_1(\kappa_L/\kappa)(\kappa/\kappa_L - 1)^2/k_B$. Note that in molecular-field theory $T_{cb}(\kappa)$ and $T_{mb}(\kappa)$ meet tangentially at the Lifshitz point. The disorder line $T_d(\kappa) = T_{cb}(\kappa) + J_1(\kappa_L/\kappa)(\kappa/\kappa_L - 1)^2/k_B$, $\kappa < \kappa_L$, does not indicate a thermodynamic phase transition but a change in the asymptotic decay of the correlation function (from exponentially damped oscillatory for $T > T_c(\kappa)$ to simple exponential for $T_d(\kappa) > T > T_{cb}(\kappa)$. The disorder line also merges tangentially at T_L with $T_{cb}(\kappa)$. Only the phase transition at the highest temperature, where the disordered (or paramagnetic) phase becomes unstable, is shown here. Commensurate–incommensurate transitions occurring at lower temperatures [4, 5] are not shown here. From Binder and Frisch [18].

behaves as

$$\chi(\vec{q}_{\parallel}, 0) = \chi_b/(1 + \xi_{\parallel}^2 q_{\parallel}^2) \qquad \chi(0, q_z) = \chi_b/(1 + \xi_{\perp}^2 q_z^4) \tag{1}$$

with $\xi_{\parallel} \propto (T - T_L)^{-\nu_{\parallel}}$, $\xi_{\perp} \propto (T - T_L)^{-\nu_{\perp}}$, with critical exponents $\nu_{\parallel} = 1/2$, $\nu_{\perp} = 1/4$ in mean-field theory [4, 5]. Of course, for an accurate description of this anisotropic critical behaviour one has to go beyond mean-field theory taking fluctuations into account, e.g. by a renormalization group treatment [6–9], but this is beyond the scope of the present paper.

Here we are concerned with the effect of a free surface on the critical behaviour of this model, and in particular, at the Lifshitz point. While surface critical behaviour of ferromagnets has been considered extensively [10–13], and also surface effects on modulated phases in isotropic systems such as block copolymer mesophases have been occasionally considered [14–17], the surface critical behaviour at uniaxial Lifshitz points has attracted attention only

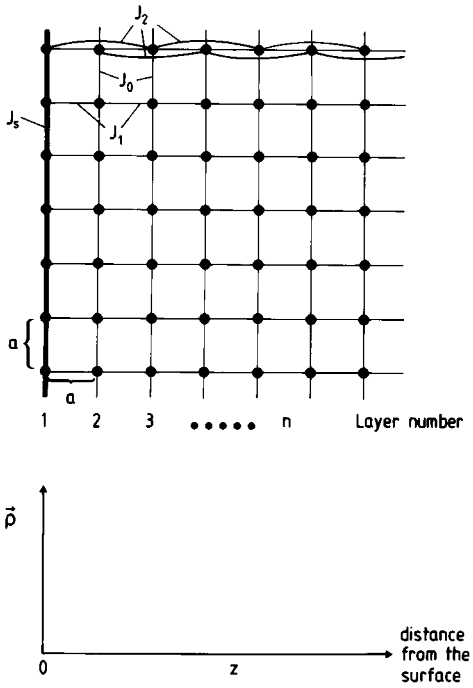

Figure 2. The cross section perpendicular to the surface plane of a semi-infinite simple cubic ANNNI model, the surface plane being oriented perpendicular to the direction where the modulation appears. Nearest-neighbour exchange constants in the surface plane are denoted as J_s, while the exchange constants in all interior planes parallel to the surface are J_0. The nearest-neighbour exchange in the z-direction perpendicular to the surface is J_1, the next-nearest-neighbour exchange in the z-direction is J_2 (it is shown explicitly in the top row only). The lattice spacing is a. In the corresponding continuum model, the lateral coordinates are denoted as $\vec{\rho}$. From Binder and Frisch [18].

recently [18, 19]. Two of the present authors (HLF and KB) have analysed the situation where the surface is oriented perpendicular to the modulation direction [18] (figure 2).

Here, we orient the free-surface plane so that it contains the modulation direction (figure 3). The anisotropy of the model renders the two surface orientations of figure 2 and figure 3 inequivalent. In particular, if a 'surface transition' [10–13] occurs in the case of figure 2 at $T_{cs}(\kappa)$, a ferromagnetic long-range order in the surface plane sets in, even for $\kappa > \kappa_L$ where the bulk has a transition to the modulated structure at $T < T_{mb}(\kappa)$. In the temperature range $T_{mb}(\kappa) < T < T_{cs}(\kappa)$ this ferromagnetic surface layer then induces a modulation perpendicular to the surface with an amplitude that decays exponentially ($\propto \exp(-z/\xi_\perp)$ where $\xi_\perp$ is the bulk correlation length in the z-direction) as one moves towards the bulk. In contrast, a surface transition in the case of figure 3 can mean the onset of either $(d-1)$-dimensional ferromagnetic or uniaxially modulated order, depending on the values of various exchange interactions j_1, j_2, J_0, J_1, and J_2 that come into play. If a modulated order in the z-direction sets in at $T_{cs}(\kappa)$, for $T < T_{cs}(\kappa)$ (but temperatures where the bulk is still disordered), a corresponding modulation will be induced in the interior layers $n = 2, 3, \ldots$, but with an exponentially decaying amplitude ($\propto \exp(-x/\xi_\parallel)$ where $\xi_\parallel$ is the bulk correlation length in the x-direction). Particularly interesting is the behaviour of the 'ordinary transition' [12, 13] (no surface transition at $T_{cs}(\kappa)$ occurs; rather the surface order is induced by the ordering of the bulk) at the Lifshitz point of the bulk: we shall see that the surface critical exponents depend on the orientation of the surface in this case.

2. Linearized molecular-field theory for the semi-infinite ANNNI model on a lattice

In molecular-field theory, every spin is aligned by the local field acting on it, so we have $\langle S_i \rangle = \tanh(H^i_{eff}/k_B T)$, and the local effective field H^i_{eff} is written as a sum of the external

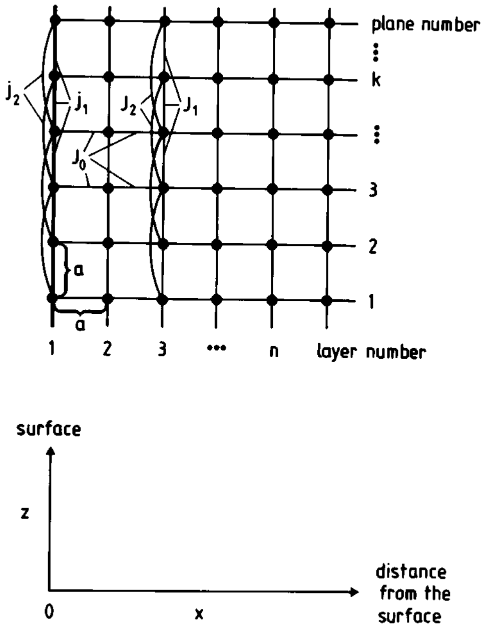

Figure 3. The cross section perpendicular to the surface plane of a semi-infinite simple cubic ANNNI model, the surface plane containing the z-direction in which the modulation appears. Nearest and next-nearest exchange constants in the z-direction are j_1, j_2 in the surface plane, and J_1, J_2 in all other planes. The (nearest-neighbour) exchange constant in all other lattice directions is J_0 (for $d \geqslant 3$ this exchange constant also occurs in the surface plane). Layers oriented parallel to the surface are labelled by an index n ($n = 1$ for the surface plane); planes oriented perpendicular to the modulation direction z are labelled by an index k.

field H^i_{ext} (it may be convenient to assume that this field is inhomogeneous, so one can consider e.g. the response to a suitably periodically modulated field) and the contributions due to the coupling to the neighbouring spins. These contributions are taken proportional to $\langle S_j \rangle$. In the region above any transition temperature and for small enough H^i_{ext}, one may linearize these molecular-field equations, which means one considers the effect of the external field H^i_{ext} in linear response. This is the only case that will be considered here.

For simplicity, we work out only the special case of a $(d = 2)$-dimensional square lattice. (This is not a serious restriction on the mean-field level, however, since molecular-field theory yields only rather trivial dependencies on dimensionality.) So the lattice sites i are labelled by two indices, for rows n and columns k, and we introduce the notation $\langle S_i \rangle = M_{n,k}$. Then the linearized mean-field equation in the bulk (i.e., $n \geqslant 2$) becomes, considering a modulated field in the bulk ($H^i_{ext} = B \exp(\mathrm{i}qka)$)

$$\begin{aligned} k_b T M_{n,k} &= B \exp(\mathrm{i}qka) + J_1(M_{n,k+1} + M_{n,k-1}) + J_2(M_{n,k+2} + M_{n,k-2}) \\ &\quad + J_0(M_{n+1,k} + M_{n-1,k}) \qquad n \geqslant 2. \end{aligned} \tag{2}$$

Here B is the amplitude of the bulk periodic field, and the special case of a bulk uniform field is recovered for $q = 0$.

In the surface layer (corresponding to $n = 1$) the couplings parallel to the surface are different. They are denoted as j_1 and j_2 (see figure 3). It is also convenient to allow for a different amplitude b of the magnetic field applied in the surface layer [10–12]. For the surface layer, the linearized molecular-field equation then becomes

$$k_B T M_{1,k} = b \exp(\mathrm{i}qka) + j_1(M_{1,k+1} + M_{1,k-1}) + j_2(M_{1,k+2} + M_{1,k-2}) + J_0 M_{2,k} \qquad n = 1. \tag{3}$$

Let

$$M_{n,k} = (m + \mu_n) \exp(\mathrm{i}qka) \tag{4}$$

where m is the 'bulk' periodic magnetization. Requiring $m + \mu_n$ to satisfy the linearized mean-field equations means

$$k_B T(m + \mu_n) = B + 2[J_1 \cos(aq) + J_2 \cos(2aq)](m + \mu_n) + J_0(2m + \mu_{n-1} + \mu_{n+1}) \tag{5}$$

and

$$k_B T(m + \mu_n) = b + 2[j_1 \cos(aq) + j_2 \cos(2aq)](m + \mu_1) + J_0(m + \mu_2). \tag{6}$$

We can assume that μ_n becomes small for large n and this allows one to extract the bulk magnetization m from equation (5):

$$m = \frac{B}{k_B T - 2[J_0 + J_1 \cos(qa) + J_2 \cos(2qa)]} = \frac{B/k_B}{T - T(q)}. \tag{7}$$

Here

$$k_B T(q) = 2[J_0 + J_1 \cos(qa) + J_2 \cos(2qa)] \tag{8}$$

is the bulk instability temperature for wavenumber q. The expression for m (equation (7)) makes sense only for temperatures which keep the denominator positive for all q. The instability of the disordered phase in the bulk occurs when T is equal to the largest $T(q)$, for a q which we denote as q_b. Maximizing $T(q)$ with respect to q gives either $q_b = 0$ (namely for $\kappa < \kappa_L$) or [18]

$$\cos(q_b a) = (4\kappa)^{-1}. \tag{9}$$

A more detailed discussion of the bulk behaviour of the ANNNI model within mean-field theory has been given by Binder and Frisch [18].

We now make the *ansatz* that the correction to the uniform magnetization decays exponentially with the distance from the surface, as is standard [10–12, 18].

$$\mu_n = \mu_1 \exp[-\Gamma(q)(n-1)] \tag{10}$$

solves equation (5) if the decay rate $\Gamma(q)$ is such that

$$\cosh[\Gamma(q)] = \{k_B T - 2[J_1 \cos(qa) + J_2 \cos(2qa)]\}/2J_0 = 1 + \frac{k_B[T - T(q)]}{2J_0}. \tag{11}$$

The amplitude of this decaying magnetization is determined by the linearized molecular-field equation at the surface layer, which serves as a boundary condition:

$$\mu_1 = \frac{b - \{k_B T - 2[j_1 \cos(qa) + j_2(\cos 2qa)] - J_0\}m}{k_B T - 2[j_1 \cos(qa) + j_2 \cos(2qa)] - J_0 \exp[-\Gamma(q)]}. \tag{12}$$

This expression can also have singularities which correspond to the surface transition if they occur at a temperature where the disordered phase is still stable in the bulk. Writing the denominator of equation (12) in analogy with equation (7) as $k_B(T - \tau(q))$ gives the instability temperature for the surface as a function of q as

$$\tau(q) = 2[j_1 \cos(qa) + j_2 \cos(2qa)] + J_0 \exp[-\Gamma(q)]. \tag{13}$$

Which type of ordering takes place depends on the functions $T(q)$ and $\tau(q)$. Let q_b be the value of q which maximizes $T(q)$ and let q_s be the value of q which maximizes $\tau(q)$. Then the following cases describe the orderings that can occur. Some special cases which one can encounter by suitable variation of the exchange constants J_1, J_2 in the bulk and j_1, j_2 in the surface are emphasized.

(1) $q_b = 0$ and $T(0) > \tau(q_s)$. Ferromagnetic bulk ordering and 'ordinary' surface critical behaviour. For $\kappa < \kappa_L$ this is similar to the standard case considered in the literature [10–13], while for $\kappa = \kappa_L$ we encounter 'ordinary' surface critical behaviour at the bulk Lifshitz point.

(2) $q_b \neq 0$ and $T(q_b) > \tau(q_s)$. Modulated bulk ordering and 'ordinary' surface critical behaviour.

(3) $q_s = 0$ and $\tau(0) > T(q_b)$. A surface transition to ferromagnetic surface ordering occurs. For $\kappa^s \equiv -j_2/j_1$ less than κ_L^s this is similar to the standard case considered in the literature [10–13], while for $\kappa^s = \kappa_L^s$ we encounter a surface version (i.e., $(d-1)$-dimensional ordering) of the Lifshitz point.

(4) $q_s \neq 0$ and $\tau(q_s) > T(q_b)$, for $\kappa^s > \kappa_L^s$. A surface transition to modulated surface ordering occurs. The behaviour is similar to that for the bulk if $q_s \to 0$ as κ^s tends to κ_L^s from above. However, for some parameters it seems possible that a discontinuous jump of q_s from a nonzero value to zero at κ_L^s occurs. This eliminates the $(d-1)$-dimensional Lifshitz-point behaviour at κ_L^s.

(5) When the surface transition at $\tau(q_s)$ and the bulk transition at $T(q_b)$ merge, we obtain the 'special transition' (also called the 'surface–bulk' multicritical point [12, 13]). This point occurs for $T(q_b) = \tau(q_s)$ in molecular-field theory. If $q_b = 0$, $q_s = 0$, and $\kappa < \kappa_L$, we have a situation similar to the standard case considered in the literature [10–13]. If both q_b and q_s are nonzero but $J_2/J_1 \neq j_2/j_1$, the physics is rather different, because different types of ordering become critical at the surface and in the bulk.

Obviously, the model considered here has a very rich phase behaviour. In the following, we shall not attempt to give an exhaustive analysis of all possible cases (note that one may also have the special case that a surface–bulk multicritical point might coincide with the Lifshitz point in the bulk, etc), but discuss only a few particularly relevant cases.

3. Surface critical behaviour near the bulk Lifshitz point

We first consider the case where $\kappa < \kappa_L$ (where $q_b = 0$) and assume surface interactions j_1, j_2 such that no surface transition occurs (as will be specified below). We then consider the response of the magnetization in the surface layer

$$M_1 = M_{1,k} = m + \mu_1 \qquad \text{independent of } k \tag{14}$$

to homogeneous bulk (B) or surface (b) fields, noting from equations (7) and (12) that

$$m = B/[k_B T - 2(J_0 + J_1 + J_2)] = B/[k_B(T - T_{cb}(\kappa))] \tag{15}$$

$$\mu_1 = \frac{b - [k_B T - 2(j_1 + j_2) - J_0]m}{k_B T - 2(j_1 + j_2) - J_0 \exp(-\Gamma)}. \tag{16}$$

Near $T = T_{cb}$ we may expand: $\exp(-\Gamma) \approx 1 - \Gamma$ and use [11] (see also reference [18]) to find $\Gamma \approx [k_B(T - T_{cb})/J_0]^{1/2}$. This yields for the surface layer susceptibility χ_1 (for definitions cf. [12])

$$\chi_1 \approx (\partial M_1/\partial B)_T \equiv \left[\frac{J_0}{k_B(T - T_{cb})}\right]^{1/2} \frac{1}{k_B T - J_0 - 2(j_1 + j_2)} \tag{17}$$

in agreement with the expected critical behaviour $\chi_1 \propto (T - T_{cb})^{-\gamma_1}$ with $\gamma_1 = 1/2$ [10–13]. Similarly, the susceptibility χ_{11} becomes

$$\chi_{11} \equiv (\partial M_1/\partial b) = [k_B T - 2(j_1 + j_2) - J_0 \exp(-\Gamma)]^{-1} \tag{18}$$

which can be expanded near $T = T_{cb}$:

$$\chi_{11} \approx [k_B T_{cb} - 2(j_1 + j_2) - J_0]^{-1} - [J_0(T - T_{cb})/k_B]^{1/2}[k_B T_{cb} - 2(j_1 + j_2 - J_0)]^{-2}. \tag{19}$$

Thus one finds a cusp-like singularity:

$$\chi_{11} \approx \chi_{11}^{crit} - \hat{\chi}_{11}(T - T_{cb})^{-\gamma_{11}} \qquad \text{with } \gamma_{11} = -1/2. \tag{20}$$

All these results, equations (17)–(20), hold only for $k_B T_{cb} - J_0 > 2(j_1 + j_2)$. When this inequality turns into an equality, we get the (ferromagnetic) surface–bulk multicritical point:

$$j_1^{SB} + j_2^{SB} = J_1 + J_2 + J_0/2. \tag{21}$$

Here the well-known result for T_{cb} was used [18]: $k_B T_{cb} = 2(J_1 + J_2 + J_0)$.

It is also interesting to work out the wavevector-dependent susceptibility $\chi_1(q)$ along the ferromagnetic line for small q. Equations (7), (12) imply for T near T_{cb}

$$\begin{aligned}\chi_1(q) &\equiv \left(\frac{\partial M_1}{\partial B \exp(\mathrm{i}qka)}\right)_T \\ &\approx \left[\frac{J_0}{k_B(T - T(q))}\right]^{1/2} \Big/ \{k_B T_{cb} - J_0 - 2[j_1 \cos(qa) + j_2 \cos(2qa)]\}.\end{aligned} \tag{22}$$

Since for small q we can expand $T(q)$ as

$$k_B T(q) \approx k_B T_{cb} - a^2 q^2 (J_1 + 4J_2) + \mathrm{o}(q^4) \tag{23}$$

we obtain

$$\chi_1(q) \approx [J_0/k_B(T - T_{cb})]^{1/2}(1 + q^2\xi_\perp^2)^{-1/2}/\{k_B T_{cb} - J_0 - 2\,[j_1 \cos(qa) + j_2 \cos(2qa)]\} \tag{24}$$

where $\xi_\perp^2 = (J_1 + 4J_2)a^2/[k_B(T - T_{cb})] \propto (T - T_{cb})^{-1}$ for $\kappa < \kappa_L$. Equation (24) shows that at $T = T_{cb}$ we obtain a power-law decay

$$\chi_1(q)\big|_{T=T_{cb}} \approx \sqrt{\frac{J_0}{a^2(J_1 + 4J_2)}}\, q^{-1} \propto q^{-2+\eta_\perp} \qquad \eta_\perp = 1. \tag{25}$$

As it should be, the scaling relation [10, 12]

$$\mu_1 = \nu_b[2 - \eta_\perp] \tag{26}$$

is satisfied for the mean-field exponents along the ferromagnetic line (remember $\nu_b = \frac{1}{2}$). Similarly,

$$\chi_{11}(q) \equiv \left(\frac{\partial M_1}{\partial_b \exp(\mathrm{i}qka)}\right)_T \simeq \{k_B T - 2[j_1 \cos(qa) + j_2 \cos(2qa)] - J_0 \exp[-\Gamma(q)]\}^{-1} \tag{27}$$

which near T_{cb} can be expanded as

$$\begin{aligned}\chi_{11}(q) &\approx \{k_B T_{cb} - 2[j_1 \cos(qa) + j_2 \cos(2qa)] - J_0\}^{-1} \\ &\quad - J_0\Gamma(q)\{k_B T_{cb} - 2[j_1 \cos(qa) + j_2 \cos(2qa)] - J_0\}^{-2}.\end{aligned} \tag{28}$$

From equation (11),

$$J_0\Gamma^2(q) \approx k_B(T - T_{cb}) + \frac{1}{2}q^2 a^2 (J_1 + 4J_2) + \mathrm{o}(q^4). \tag{29}$$

Thus at T_{cb} the singular part of $\chi_{11}(q)$ scales as $\chi_{11}^{sing}|_{T=T_{cb}} \propto q = q^{-1+\eta_\parallel}$ which yields the well-known result $\eta_\parallel = 2$ [10–12]. Thus the scaling relation [10–12]

$$\gamma_{11} = \nu_b(1 - \eta_\parallel) \tag{30}$$

is also fulfilled along the whole ferromagnetic line, $0 \leqslant \kappa < \kappa_L$, and the exponents all have their standard values. Only amplitude prefactors depend on κ, as expected.

We next consider the modulated phase, $\kappa > \kappa_L$, and obtain the wavevector-dependent response functions for $q = q_b$, assuming that q_b is small enough that we may approximate $\cos q_b \approx 1 - q_b^2/2$, i.e. $q_b = \sqrt{2}\sqrt{1-\kappa_L/\kappa}$ [18]. Near $T = T_{mb} = T(q_b)$ we again have $\Gamma(q_b) \approx [k_B(T - T_{mb})/J_0]^{1/2}$ and hence the response functions for modulated order become

$$\chi_1^m \equiv (\partial M_1/\partial[B\exp(\mathrm{i}q_b ka)])_T = \partial(m+\mu_1)/\partial B \\ \approx \left(\frac{J_0}{k_B(T-T_{mb})}\right)^{1/2} \\ \times \left\{k_B T_{mb} - J_0 - 2[j_1\cos(q_b a) + j_2\cos(2q_b a)] + J_0\Gamma(q_b)\right\}^{-1} \tag{31}$$

and

$$\chi_{11}^m \equiv (\partial M_1/\partial[b\exp(\mathrm{i}q_b ka)]) \\ = \{k_B T - 2[j_1\cos(q_b a) + j_2\cos(2q_b a)] - J_0 + J_0\Gamma(q_b)\}^{-1}\,. \tag{32}$$

These results yield the same type of singularity for the surface critical behaviour along the transition line to the modulated phase as for the ferromagnetic transition:

$$\gamma_1^{(m)} = 1/2 \qquad \gamma_{11}^{(m)} = -1/2. \tag{33}$$

Considering the wavevector-dependent response for $q \neq q_b$ and expanding in $q - q_b$, one can also show that $\eta_\perp^{(m)} = 1$, $\eta_\parallel^{(m)} = 2$ and the scaling relations equations (26), (30) continue to hold.

From the phase diagram (figure 1) it follows that we can readily obtain the critical behaviour at the Lifshitz point letting $\kappa = \kappa_L = 1/4$ and $q_b = 0$. Thus we see that

$$\chi_1^L \approx \left(\frac{J_0}{k_B(T-T_L)}\right)^{1/2} \Big/ \{k_B T_L - J_0 - 2(j_1+j_2)\} \qquad \text{i.e. } \gamma_1^L = 1/2 \tag{34}$$

$$\chi_{11}^L = \{k_B T - 2(j_1+j_2) - J_0 + J_0\Gamma\}^{-1} \qquad \text{i.e. } \gamma_{11}^L = -1/2. \tag{35}$$

While these exponents are the same as along the ferromagnetic line, the exponents $\eta_\perp^L$, $\eta_\parallel^L$ differ. This is obtained from an expansion analogous to equation (29). The term proportional to q^2 vanishes and one must include a term proportional to q^4. For $\kappa = \kappa_L$,

$$k_B T(q) = k_B T_L + \frac{1}{12}(aq)^4(J_1 + 16J_2) + \mathrm{o}(q^6). \tag{36}$$

Hence the wavevector-dependent surface layer susceptibilities at the Lifshitz point become

$$\chi_1^L(q) = \sqrt{\frac{J_0/k_B}{T-T_L}}\frac{1}{\sqrt{1+q^4\xi_\perp^4}} \Big/ \{k_B T_L - J_0 - 2[j_i\cos(aq) + j_2\cos(2aq)]\} \tag{37}$$

where

$$\xi_\perp = a\left(\frac{J_1}{4k_B}\right)^{1/4}(T-T_L)^{-1/4} \qquad \xi_\perp \propto (T-T_L)^{-\nu_\perp^L} \qquad \nu_\perp^L = 1/4 \tag{38}$$

and

$$\chi_{11}^L(q) \approx \{k_B T_L - 2[j_1\cos(qa) + j_2\cos(2qa)] - J_0\}^{-1} \\ - J_0^{1/2}[k_B(T-T_L) - q^4a^4(J_1+16J_2)/12]^{1/2} \\ \times \{k_B T_L - 2[j_1\cos(qa) + j_2\cos(2qa)] - J_0\}^{-2} + \cdots. \tag{39}$$

These results show that for $T = T_L$ the q-dependence is

$$\chi_1^L(q) \propto q^{-2} \qquad \chi_{11}^{L,sing}(q) \propto q^{+2} \tag{40}$$

i.e., the exponents $\eta_\perp^L$, $\eta_\parallel^L$ are ($\chi_1^L(q) \propto q^{-2+\eta_\perp^L}$, $\chi^{L,sing}(q) \propto q^{-1+\eta_\parallel^L}$)

$$\eta_\perp^L = 0 \qquad \eta_\parallel^L = 3. \tag{41}$$

These are exactly the values required to satisfy the scaling relations

$$\gamma_1^L = \nu_\perp^L(2 - \eta_\perp^L) = \frac{1}{4} \times 2 = \frac{1}{2} \qquad \gamma_{11}^L = \nu_\perp^L(1 - \eta_\parallel^L) = \frac{1}{4} \times (-2) = -\frac{1}{2}. \tag{42}$$

We emphasize at this point that for the orientation of the surface perpendicular to the z-axis (where the competing interactions occur) a completely different set of exponents has been found, namely [18]

$$\gamma_1^L = 1/2 \qquad \gamma_{11}^L = -1/4 \qquad \eta_\parallel^L = 3/2 \qquad \eta_\perp^L = 1. \tag{43}$$

Considering here also a q-vector oriented parallel to the surface, it is clear that the correlation length $\nu_\parallel^L = 1/2$ rather than $\nu_\perp^L = 1/4$ has to be used in the scaling relations, equations (26), (30), which are then also fulfilled. Comparing equations (34), (35), (41) with equation (43) shows the most important result of the present work, namely that the surface critical exponents at a uniaxial Lifshitz point depend on the orientation of this axis relative to the surface.

4. Surface transitions

We return to the case $\kappa < \kappa_L$ where $q_b = 0$ and also assume $q_s = 0$, but now we allow for the case that has been excluded in the previous section, namely $k_B T_{cb} - J_0 < 2(j_1 + j_2)$: the negative sign of the denominator in equation (17) then signals that this equation is no longer valid. Instead a surface transition has occurred, at a critical temperature T_{cs} which is given by the implicit equation

$$k_B T_{cs} = 2(j_1 + j_2) + J_0 \exp\{-\Gamma(T_{cs})\}. \tag{44}$$

All susceptibilities $\chi_1(T)$ and $\chi_{11}(T)$ have simple Curie–Weiss singularities there, familiar from bulk critical points in the mean-field approximation. This is seen via the expansion

$$\exp\{-\Gamma(T)\} \cong \exp\{-\Gamma(T_{cs})\}\left\{1 - (T - T_{cs})\left(\frac{\mathrm{d}\Gamma}{\mathrm{d}T}\right)_{T=T_{cs}}\right\} \tag{45}$$

which yields, together with equation (18)

$$\chi_{11} = [k_B(T - T_{cs})]^{-1} \times \left\{1 + J_0 \exp[-\Gamma(T_{cs})]\left(\frac{\mathrm{d}\Gamma}{\mathrm{d}T}\right)_{T=T_{cs}}\right\}^{-1} \qquad \text{for } j_1 + j_2 > J_1 + J_2 + \frac{J_0}{2} \tag{46}$$

and a similar result applies for χ_1. These results do not differ in any significant way from the surface critical behaviour of the nearest-neighbour Ising ferromagnet; they hold for all $\kappa < \kappa_L$ but not including the Lifshitz point. However, since the above assumption that $q_b = 0$ for $T > T_{cb}$ holds only underneath the disorder line, $T < T_d(\kappa)$ [20], and $T_d(\kappa)$ merges with $T_{cb}(\kappa)$ at the Lifshitz point [18]; cf. figure 1.

More interesting is the case where a modulated phase appears at the surface before any order appears at the bulk. We are not treating this problem in full generality, but focus only on the situation where $q_s a \ll 1$, so $\cos(q_s a)$ can be expanded:

$$\tau(q_s) \approx 2(j_1 + j_2) + J_0 - a^2 q_s^2 (j_1 + 4j_2) + \frac{a^4 q_s^4}{12}(j_1 + 16 j_2) - J_0 \Gamma(q_s) + \frac{1}{2} J_0 \Gamma^2(q_s) \tag{47}$$

where

$$\Gamma(q_s) = J_0^{-1/2}[k_B(T - T_{cb}) + a^2 q_s^2 (J_1 + 4J_2) - \frac{1}{12} a^4 q_s^4 (J_1 + 16J_2)]^{1/2}.$$

However, care is necessary in the proper treatment of $\Gamma(q_s)$: when $T \to T_{cb}$ the term $k_B(T - T_{cb})$ will always get smaller than the subsequent terms even for very small q_s, and therefore in this limit the square root cannot be expanded in a power series in q_s. Such an expansion is possible only when T_{cs} is sufficiently larger than T_{cb} that $k_B(T_{cs} - T_{cb})$ for all q of interest is the dominating term under the square root. In this limit one gets

$$\begin{aligned}
\tau(q) \approx{} & 2(j_1 + j_2) + J_0 - a^2 q^2 (j_1 + 4j_2) + \frac{a^4 q^4}{12}(j_1 + 16 j_2) - J_0 \left[\frac{k_B(T_{cs} - T_{cb})}{J_0}\right]^{1/2} \\
& - \frac{1}{2}\left[\frac{J_0}{k_B(T_{cs} - T_{cb})}\right]^{1/2} (J_1 + 4J_2)(a^2 q^2) \\
& + \left\{\frac{1}{24}\left[\frac{J_0}{k_B(T_{cs} - T_{cb})}\right]^{1/2} (J_1 + 16J_2) \right. \\
& \left. + \frac{1}{8J_0}\left[\frac{J_0}{k_B(T_{cs} - T_{cb})}\right]^{3/2} (J_1 + 4J_2)^2 \right\} a^4 q^4 \\
& + \frac{1}{2} k_B(T_{cs} - T_{cb}) + \frac{1}{2}(J_1 + 4J_2)(a^2 q^2) - \frac{1}{24}(J_1 + 16J_2)(a^4 q^4).
\end{aligned} \tag{48}$$

Then q_s is found from the condition $\mathrm{d}\tau(q)/\mathrm{d}q = 0$ (and $\mathrm{d}^2\tau(q)/\mathrm{d}q^2|_{q_s} < 0$). This yields (note that both the numerator and the denominator of the following expression must be negative)

$$\begin{aligned}
a^2 q_s^2 ={} & \left\{2(j_1 + 4j_2) + \left[\frac{J_0}{k_B(T_{cs} - T_{cb})}\right]^{1/2} (J_1 + 4J_2) - (J_1 + 4J_2)\right\} \Big/ \left\{\frac{1}{3}(j_1 + 16 j_2) \right. \\
& + \frac{1}{6}\left[\frac{J_0}{k_B(T_{cs} - T_{cb})}\right]^{1/2} (J_1 + 16J_2) + \frac{1}{2J_0}\left[\frac{J_0}{k_B(T_{cs} - T_{cb})}\right]^{3/2} \\
& \left. \times (J_1 + 4J_2)^2 - \frac{1}{6}(J_1 + 16J_2)\right\}.
\end{aligned} \tag{49}$$

Thus we conclude that the surface Lifshitz point, where $q_s \to 0$, is given by the condition

$$2(j_1 + 4j_2) = (J_1 + 4J_2)\left\{1 - \left[\frac{J_0}{k_B(T_{cs} - T_{cb})}\right]^{1/2}\right\} \tag{50}$$

where T_{cs} is given by the solution of equation (44). Since the expansion that we have used requires $\Gamma(q_s) \ll 1$, $\Gamma(q_s = 0) \approx [k_B(T - T_{cb})/J_0]^{1/2}$, we see that the curly bracket in equation (50) is large and negative, while the term $J_1 + 4J_2$ changes sign at the Lifshitz point of the bulk. So for $\kappa < \kappa_L$ where $J_1 + 4J_2 > 0$, we can have a surface Lifshitz point only if $|j_1 + 4j_2| \gg J_1 + 4J_2$ and $j_1 + 4j_2$ is negative. As a result, the ratio $\kappa_s = j_2/j_1$ must be more negative than the bulk value $\kappa_L = -1/4$, in order to allow a modulated phase on the surface of a ferromagnet. The actual transition temperature to the phase with $q_s > 0$ is found by inserting equation (49) into equation (48). The resulting expression is rather clumsy and hence is not reproduced here.

We now consider the inverse limit where $T_{cs} \to T_{cb}$, being interested in the behaviour where a surface transition to a modulated phase merges with the bulk (ferromagnetic) transition. Then for $J_1 + 4J_2 > 0$ we can approximate $\Gamma(q)$ as

$$\Gamma(q) \approx aq\sqrt{(J_1 + 4J_2)/J_0} \tag{51}$$

and instead of equation (48) we find

$$\tau(q) \approx 2(j_1 + j_2) + J_0 - a^2q^2(j_1 + 4j_2) + \frac{a^4q^4}{12}(j_1 + 16j_2) \\ - aq\sqrt{J_0(J_1 + 4J_2)} + \frac{1}{2}a^2q^2(J_1 + 4J_2). \qquad (52)$$

Due to the term $aq\sqrt{J_0(J_1 + 4J_2)}$ we recognize that $\tau(q)$ always decreases with increasing q near $q = 0$, irrespective of the values of the parameters, so there is always a local maximum at $q = 0$. (Note that we have defined q non-negative; therefore this maximum really appears in this treatment as a boundary effect, and cannot be identified from $\mathrm{d}\tau(q)/\mathrm{d}q = 0$.) On the other hand, the solution of $\mathrm{d}\tau(q)/\mathrm{d}q = 0$ may lead to a maximum of $\tau(q)$ at some nonzero q_s, and if $\tau(q_s) > \tau(0)$ the solution q_s yields the physically relevant case. If we change the parameters j_1, j_2, J_1, J_2 such that we reach the situation where

$$\tau(q_s) = \tau(0) \qquad (53)$$

then the solution with $q_s > 0$ disappears discontinuously and the solution with $q_s = 0$ takes over. Since q_s cannot vanish smoothly when $T_{cs} = T_{cb}$, a surface bulk multicritical point which simultaneously is a surface Lifshitz point (but not a bulk Lifshitz point) cannot occur.

The value q_s^{crit} for which equation (53) is fulfilled and the surface transition line T_{cs} hits the bulk transition temperature T_{cb} (remember, we discuss only the case $\kappa < \kappa_L$ here, i.e. $J_1 + 4J_2 > 0$) is easily obtained as follows. First we note that a necessary condition for the expansion equation (52) to make sense is

$$j_1 + 4j_2 - \frac{1}{2}(J_1 + 4J_2) < 0 \qquad j_1 + 16j_2 < 0. \qquad (54)$$

Only then can we expect a maximum of $\tau(q)$ for small but positive q, while if $j_1 + 16j_2 > 0$, $\tau(q)$ would increase for large q, i.e. the expansion then does not make any sense. If $j_1 + 4j_2 - \frac{1}{2}(J_1 + 4J_2) > 0$, all q-dependent terms in equation (52) would have the same sign, i.e. $\tau(q)$ would uniformly decrease as q increases. Using equations (52), (53) together with $\mathrm{d}\tau(q)/\mathrm{d}q = 0$ yields

$$(aq_s^{crit})^2 = \left[\frac{1}{2}(J_1 + 4J_2) - (j_1 + 4j_2)\right] \Big/ [4|j_1 + 16j_2|]. \qquad (55)$$

Note that at the same time j_1, j_2 must satisfy equation (21), and thus the three parameters q_s, j_1^{SB}, j_2^{SB} are uniquely determined from the three equations $\mathrm{d}\tau(q)/\mathrm{d}q = 0$, equation (21), and equation (53), respectively. However, in the limit where equations (48), (49) are valid, one has $\mathrm{d}^2\tau(q)/\mathrm{d}q^2 > 0$ for $q = 0$, i.e. $q = 0$ is a minimum, and the condition $\tau(0) = \tau(q)$ would simply yield $q = \sqrt{2}q_s$. This cannot be solved together with $\mathrm{d}\tau(q)/\mathrm{d}q = 0$: $\tau(q_s) > \tau(0)$ as long as $q_s > 0$. However, when at $T = T_{cs}$ one has

$$(j_1 + 4j_2) + \frac{1}{2}(J_1 + 4J_2)\left\{\left[\frac{J_0}{k_B(T_{cs} - T_{cb})}\right]^{1/2} - 1\right\} > 0$$

so $q_s = 0$ is a maximum of $\tau(q)$ and the solution found in equation (49) would be a minimum. Another maximum at a value of q that tends to q_s^{crit} as given by equation (55) for $T_{cs} \to T_{cb}$ occurs if equation (54) is fulfilled. For a discussion of this situation a more accurate analysis of $\tau(q)$ in equation (13) would be required. Figure 4 shows the possible behaviour of $\tau(q)$ schematically.

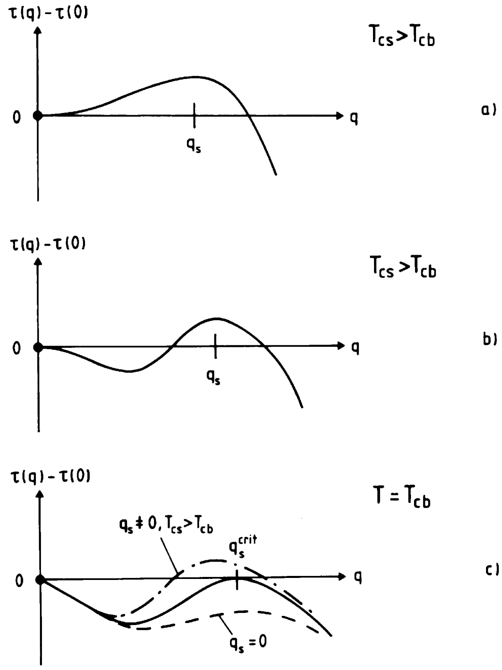

Figure 4. A schematic sketch of the behaviour of $\tau(q) - \tau(0)$ as a function of q for three different cases leading to modulated order at the surface of a ferromagnet. Cases (a), (b) correspond to the case $T_{cs} > T_{cb}$ and $(j_1 + 4j_2) + \frac{1}{2}(J_1 + 4J_2)\{[J_0/k_B(T_{cs} - T_{cb})]^{1/2} - 1\} < 0$ (a) or >0 (b), respectively, while case (c) corresponds to $T = T_{cb}$ and $(j_1 + 4j_2) - \frac{1}{2}(J_1 + 4J_2) < 0$, indicating how q_s^{crit} (equation (55)) can be found by suitable variation of j_2/j_1 at fixed $j_1 + j_2$.

5. The continuum model

As is well known [3–13], molecular-field theory is a modest first step in the description of critical phenomena, and for a treatment of fluctuations one either has to resort to Monte Carlo simulations (which are somewhat cumbersome for the ANNNI model even in the bulk [4, 5]) or to renormalization group expansions [6–9, 13]. The latter need a continuum version of molecular-field theory as their starting point. For completeness, we formulate here the continuum version of our model, although a renormalization group treatment is beyond the scope of our work.

As in [18], we transform the difference equations into a differential equation with the help of the expansion ($\mu_n \equiv \mu(z)$)

$$\mu(z \pm a) = \mu(z) \pm a \, \mathrm{d}\mu/\mathrm{d}z + \frac{1}{2}a^2 \frac{\mathrm{d}^2\mu}{\mathrm{d}z^2} + \cdots \tag{56}$$

so equation (5) becomes

$$\{2[J_0 + J_1 \cos(aq) + J_2 \cos(2aq)] - k_B T\}\mu(z) + \frac{1}{2}a^2 J_0 \frac{\mathrm{d}^2\mu}{\mathrm{d}z^2} = 0 \tag{57}$$

where we have used equation (7) to eliminate the bulk magnetization m. A decaying exponential solution away from the boundary which we now shift to $z = 0$ is

$$\mu(z) = \mu(0) \exp[-\Gamma(q) z/a] \tag{58}$$

and substituting equation (58) into (57) yields

$$J_0\Gamma^2(q) = 2\{2[J_0 + J_1\cos(qa) + J_2\cos(2qa)] - k_BT\}. \tag{59}$$

Near T_{cb} where in equation (11) one may write $\cosh[\Gamma(q)] \approx 1 + \frac{1}{2}\Gamma^2(q)$ one sees that equations (11) and (59) are equivalent, while further away from T_{cb} these equations differ [18].

The constant $\mu(0) = \mu_0$ can be determined from the boundary condition at $z = 0$. Expanding μ_2 in equation (6) as $\mu(a) = \mu(0) + a(\mathrm{d}\mu/\mathrm{d}z)|_{z=0}$ yields

$$k_BT\mu_0 = 2[j_1\cos(qa) + j_2\cos(2qa)]\mu_0 + J_0\mu_0 + J_0a(\mathrm{d}\mu/\mathrm{d}z)_{z=0} + K \tag{60}$$

where we have used the abbreviation

$$K = b + [J_0 + 2j_1\cos(qa) + 2j_2\cos(2qa) - k_BT]m. \tag{61}$$

Equation (60) is a boundary condition linking $\mu_0 = \mu(z = 0)$ and $(\mathrm{d}\mu/\mathrm{d}z)_{z=0}$ [10–13], which is different from the case where the z-axis is oriented perpendicular to the surface. The differential equation analogous to equation (57) then contains a term proportional to $\mathrm{d}^4\mu/\mathrm{d}z^4$ as well, and two boundary conditions including both terms in $(\mathrm{d}\mu/\mathrm{d}z)_{z=0}$ and $(\mathrm{d}^2\mu/\mathrm{d}z^2)_{z=0}$ required [18].

Since equation (58) implies $(\mathrm{d}\mu/\mathrm{d}z)_{z=0} = -\mu(0)\Gamma(q)/a$, one readily finds from equation (60) that

$$\mu_0 = K/(k_BT - \tau_{cont}(q)) \tag{62}$$

which is the continuum analogue of equations (12), (13) but with

$$\tau_{cont}(q) = 2[j_1\cos(qa) + j_2\cos(2qa)] - J_0[1 - \Gamma(q)]. \tag{63}$$

Again we find agreement with the result of the difference equation, equation (12), if we expand $\exp[-\Gamma(q)] \approx 1 - \Gamma(q)$, which is appropriate for T close to T_{cb}. As usual, the condition for the applicability of the continuum approximation is that the correlation length ξ_b is much larger than the lattice spacing.

Of course, in the basic molecular-field equation $H^i_{eff}/k_BT = \mathrm{arctanh}(\langle S_i\rangle)$ one must also include the leading nonlinear term resulting from $\mathrm{arctanh}(x) \approx x + x^3/3$ which yields a term $\mu^3(z)$ to be added in equation (57), in order that the standard Ginzburg–Landau equation [10–13] for surface critical phenomena is obtained.

6. Conclusions

In this study we have extended previous work on surface effects on the critical behaviour of the ANNNI model, where the z-axis along which nearest- and next-nearest-neighbour exchange (J_1, J_2) compete was oriented perpendicular to the surface, by considering the alternative case where the z-axis is contained in the surface plane. We have allowed for different interactions (j_1, j_2) along the z-axis in the surface plane, and we have shown that—within the mean-field theory—surface transitions may occur at temperatures exceeding the bulk transition temperature. We have also shown that modulated surface structures occur on the surface of a ferromagnet, and paid attention to the occurrence of surface Lifshitz points as well as to the possibility that the wavenumber q_s of the surface modulation jumps to zero discontinuously when a critical value q_s^{crit} is reached.

Pronounced deviations from mean-field behaviour due to statistical fluctuations are expected: two-dimensional modulated phases belong to the universality class of the two-dimensional XY-model and hence lack true long-range order. The surface transition to modulated structures hence should be of the Kosterlitz–Thouless type, and no Lifshitz point occurs in $d = 2$ dimensions [4, 5] at nonzero temperature. As a result, no surface Lifshitz points are expected to exist either.

Thus we feel that our most physically relevant results concern the surface effects on the bulk Lifshitz point. We have obtained the exponents γ_1, γ_{11}, $\eta_\perp$, $\eta_\parallel$ and we have shown that they satisfy the expected scaling relations. We expect that these scaling relations hold beyond mean-field theory, although the actual values of the exponent are unknown when one goes beyond mean-field theory. (Note that the upper critical dimension for uniaxial Lifshitz points is $d_u = 4.5$ and thus somewhat larger differences from mean-field values are expected for $d = 3$ than for ordinary critical phenomena for which $d_u = 4$ [4–9].) An important qualitative consequence of the anisotropy of the model, which is expected to apply also beyond mean-field theory, is the fact that the surface critical exponents depend on the orientation of the surface relative to the distinct axis.

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