A study of the \((m, d, N) = (1, 3, 2)\) Lifshitz point and of the three-dimensional XY universality class by high-temperature bivariate series for the XY models with anisotropic competing interactions

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Abstract

High-temperature bivariate expansions have been derived for the two-spin correlation-function in a variety of classical lattice XY (planar rotator) models in which spatially isotropic interactions among first-neighbor spins compete with spatially isotropic or anisotropic (in particular uniaxial) interactions among next-to-nearest-neighbor spins. The expansions, calculated for cubic lattices of dimension \(d = 1, 2\) and \(3\), are expressed in terms of the two variables \(K_1 = J_1/kT\) and \(K_2 = J_2/kT\), where \(J_1\) and \(J_2\) are the nearest-neighbor and the next-to-nearest-neighbor exchange couplings, respectively. This report deals in particular with the properties of the \(d = 3\) uniaxial XY model (ANNNXY model) for which the bivariate expansions have been computed through the 18-th order, thus extending by 12 orders the results so far available and making a study of this model possible over a wide range of values of the competition parameter \(R = J_2/J_1\). Universality with respect to \(R\) on the critical line separating the para- and the ferro-magnetic phases can be verified, and at the same time the very accurate determination \(\gamma = 1.3177(5)\) and \(\nu = 0.6726(8)\) of the critical exponents of the susceptibility and of the correlation-length, in the three-dimensional XY universality class, can be achieved. For the exponents at the multi-critical \((m, d, N) = (1, 3, 2)\) Lifshitz point the estimates \(\gamma_l = 1.535(25), \nu_\perp = 0.805(15)\) and \(\nu_\parallel = 0.40(3)\) are obtained. Finally, the susceptibility exponent is estimated along the boundary between the disordered and the modulated phases.

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I. INTRODUCTION

Bivariate high-temperature (HT) and, in some cases, low-temperature (LT) series expansions have been derived in the last four decades only for very few lattice spin models with interactions extending beyond nearest-neighbor (nn) sites. In principle, undertaking such calculations should be of permanent interest, because the analytic approximations based on the series coefficients can make a large part of the (at least) bidimensional interaction-parameter space easily accessible to analysis above (respectively below) the transition temperature. In practice, however, the presence of the next-to-nearest neighbor (nnn) interactions makes the derivation of adequately long expansions by the conventional graph techniques, very laborious. As a consequence, only data at relatively low orders and therefore of limited use, have been so far available for a handful of non-trivial models and the less tedious and more flexible approach to the study of these systems by stochastic simulations has largely prevailed in the literature, despite its forced limitation to a coarse-grained survey of the interaction-parameter space and the convergence problems often met with in particular regions of the phase diagrams.

The earliest studies of short two-variable \(^1\) (or, in some cases, even three-variable \(^2\) series, particularly in the case of \(N\)-vector spin systems, helped to substantiate and qualify the critical universality hypothesis in its statement concerning the independence of the critical exponents (and of the other universal quantities) on the range of the interaction. Decisive progress in the study of this property was achieved much later with the advent of simulation algorithms optimized \(^3\) for long-range interactions. It was however already known that, when the nnn interactions compete with the nn interactions, frustration occurs (in absence of disorder) and, as initially shown in the mean-field approximation \(^4,5\), produces “special effects” \(^6\). The physically interesting new features include:

a) the formation of spatially modulated phases, i.e. spin configurations in which the order parameter varies periodically in space with a characteristic modulation wave-vector depending on the temperature and the ratio of the competing exchange couplings \(^4,5,6,7,8,9,10,11,12,13,14,15,16,17,18\);

b) the occurrence of a special multi-critical point \(^8\), called Lifshitz point (LP), at which the HT disordered phase meets both the LT spatially-uniform ordered phase and the LT spatially-modulated ordered phase(s).

Competing interactions and LP’s are present in a variety of magnetic, ferroelectric, polymeric, liquid crystal systems, in microemulsion models etc., which sometimes have not yet been studied in complete detail theoretically \(^12,13,14,15,16,17,18,19,20,21\) or experimentally \(^22\) and continue to be actively explored. It is also worth to mention that within the lattice approach to Euclidean quantum field theory there is a continuing interest into models of the same or analogous structure \(^22,23\), which are expected to show a faster approach to the continuum limit.

II. THE SPIN MODELS

We begin with a general description of several systems of \(N\)-vector spins with \(nn\) and \(nnn\) interactions on simple-cubic lattices of spatial dimensions \(d = 1, 2\) and \(3\), in zero external field, for which we have computed from the beginning or extended the bivariate HT series. Then we shall discuss a first brief analysis of a small sample of the large body of data so far accumulated, referring to a particular three-dimensional system of spins with \(N = 2\)
components, i.e. to a classical XY (or planar rotator) model. The case of general \( N \) will be the subject of forthcoming work.

We have derived bivariate HT expansions for:

\( i \) a class of \( d \)-dimensional models with isotropic interactions \( J_1 \) among \( nn \) spins and isotropic (or anisotropic) interactions \( J_2 \) among \( nnn \) spins separated by two lattice spacings along \( m \leq d \) lattice axes. They are described by the Hamiltonian:

\[
H_{nnn}\{v\} = -2J_1 \sum_{nn} \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}') - 2J_2 \sum_{nnn} \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}')
\]

(1)

where we have denoted by \( \vec{v}(\vec{r}) \) a \( N \)-component classical spin vector of unit length situated at the lattice site \( \vec{r} \). In eq. (1) the first sum, extended to \( nn \) spins, describes the interactions among the spins at \( \vec{r} \) and the spins at the sites \( \vec{r}' = \vec{r} \pm \hat{x}_i \) with \( \hat{x}_i \) a unit lattice vector in the positive \( x_i \) direction. The second sum describes the interactions among the spin at \( \vec{r} \) and the spins at the sites \( \vec{r}' = \vec{r} + 2\hat{x}_i \) with \( i = 1, \ldots, d \) in the isotropic \( d - axial \) case (i.e. in which spins separated by two spacings interact along all lattice axes), whereas \( i \) takes only the values \( i = d - m + 1, \ldots, d \) in the anisotropic \( m - axial \) case, with \( m < d \). In this report we study in detail only the most interesting case of the \( m = 1 \) model in \( d = 3 \), which is sometimes denoted also as the three-dimensional ANNNXY model.

\( ii \) a class of models with isotropic or anisotropic interactions \( J_1 \) among \( nn \) spins and \( J_2' \) among (geometric) second-neighbor \( (sn) \) spins (sometimes also called \( J_1 - J_2 \) model or model with crossing bonds) described by the following Hamiltonian:

\[
H_{sn}\{v\} = -2J_1 \sum_{nn} \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}') - 2J_2' \sum_{sn} \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}')
\]

(2)

The first sum in eq. (2) has the same meaning as in eq. (1), while the second sum extends to \( sn \) spins and describes the coupling of the spin at \( \vec{r} \) with the spins at the sites \( \vec{r}' = \vec{r} \pm \hat{x}_i + \hat{x}_j \) and \( \vec{r}' = \vec{r} + \hat{x}_i - \hat{x}_j \) with \( i < j = 1, \ldots, d \) (i.e. the \( sn \) interaction acts along the diagonals of the elementary plaquettes).

In eq. (1) we have denoted by \( J_1 \) and \( J_2 \) the \( nn \) and the \( nnn \) exchange interaction constants respectively. We shall denote by \( R = J_2/J_1 \) their ratio, which measures the degree of competition of the couplings and therefore is usually called competition parameter. In eq. (2) \( J_2' \) denotes the \( sn \) interaction constant and we set \( R' = J_2'/J_1 \). Our HT expansions are expressed in terms of the two variables \( K_1 = \beta J_1 \) and \( K_2 = \beta J_2 \) \( (K_2' = \beta J_2') \), with \( \beta = 1/kT \), \( k \) the Boltzmann constant and \( T \) the temperature.

By the same techniques used in this paper, expansions can be derived also for a much wider variety of systems, but here we shall not be concerned with this possibility.

In the case of the \( 1 - axial \) XY model in \( d = 3 \) studied in this report, our series extend through the 18-th order (altogether 171 nonzero coefficients in the case of the susceptibility) the existing\(^{25}\) sixth-order results (21 nonzero coefficients, respectively). The extensions obtained for the other models described in \( i \) and \( ii \) are comparable.

The complete set of our series coefficients is too extensive to print here. We shall however upload in the hep-lat archive a separate report containing a large sample of these data, including the correlation functions between \( nn \) and \( sn \) (or \( nnn \)) spins, the energy density, the susceptibility and a few correlation moments for the models we have studied.

It is fair to note that, in spite of their high computational complexity and cost, our bivariate series still reach a length which may still be considered only “moderate” with respect to the current best standards for univariate HT expansions. For example, as far
as the accuracy of the numerical output of their analysis is concerned, they are not yet comparable with the 25-th order univariate series computed in the case of three-dimensional scalar spin systems with \( nn \) interactions only, (such as the Ising model with generic spin or the lattice Euclidean scalar field), or with the 26-th order series derived in the case of the two-dimensional XY model with \( nn \) interactions on the square lattice. However, if the comparison is limited to the bivariate series calculated until now for the systems \( i) \) and \( ii) \) (see below), our expansions seem to be already non-trivial enough to justify an update of the few existing HT studies or a first analysis of the data so far unavailable.

We have studied the expansions of observables defined in terms of two-spin correlations, as functions of \( K_1 \) at fixed values of \( R \), using, for the moment, only the established single-variable methods of series analysis, namely Padè approximants (PA) or inhomogeneous differential approximants (DA), and, adopting protocols of analysis well tested in earlier papers, we have indeed produced reasonably accurate results which can complement or improve those from different approaches. The choice of single variable methods of numerical analysis, which might perhaps be considered partly responsible of the limited accuracy of our numerical results, was dictated only by simplicity, but it is likely that now the HT series are long enough to deserve the additional effort of an analysis by tools more powerful and better suited to describe bivariate critical behavior, such as the partial-differential approximants or even some simpler two-variable generalization of PA.

For \( N > 1 \), the lower critical dimension of the so called \( (m, d, N) \) Lifshitz point occurring in a \( m-axial \) \( N \)-vector system in \( d \) dimensions, is \( d_l(m) = 2 + m/2 \), while the upper critical dimension is \( d_u(m) = 4 + m/2 \). Therefore one has to expect that only in dimension \( d > 2 \), for the \( 1-axial \) model, a LP will show up at \( T_{LP} > 0 \) with a non-classical critical behavior. Thus we can use our HT series for the three-dimensional ANNNXY model to locate its LP and to obtain estimates of its critical exponents, for which some predictions from other approximation methods already exist.

More generally, it is also of interest to analyze the behavior of the series as functions of \( R \) all along the critical line separating the paramagnetic from the ordered phases. In particular, along the critical line between the disordered and the ferromagnetic phases we can take advantage in our analysis of the old suggestion that the accuracy in the determination of universal critical parameters of a given \( N \)-vector model, such as critical exponents and universal amplitude ratios, can be significantly improved by extending the analysis to a one-parameter family of models belonging to the same universality class. One should then simply “tune” the family parameter in order to minimize or, if possible, to suppress the amplitudes of the (non-universal) leading non-analytic corrections to scaling in the observables used to evaluate the critical parameters. This procedure can be implemented by a Monte Carlo (MC) method only, by HT-series assisted MC, or by HT series only, and has been successfully applied in a variety of cases involving \( nn \) and local spin interactions, so far with a single exception for the spin-1/2 Ising model on the simple-cubic lattice. In this case, a high-precision MC analysis showed that turning on an isotropic ferromagnetic coupling beyond \( nn \) results into a considerable decrease of the leading correction-to-scaling amplitudes. Unfortunately, this simulation study had to be restricted to a single well-guessed value of the \( nnn \) coupling, because “tuning” the additional (irrelevant) interaction to search for its best value, was too time-consuming. Now, in the case of the \( N \)-vector model with \( N = 2 \), our expansions are sufficiently extended to produce accurate analytic approximations enabling us to determine in a straightforward way the optimal value of the irrelevant \( nnn \) coupling within a fair approximation.
The LP can be located accurately and the exponents of the susceptibility and of the transverse correlation-length can be determined with fair precision, while the exponent of the parallel correlation-length can be somewhat less accurately estimated. We have also examined the critical behavior of the susceptibility along the branch of the critical line between the disordered and the modulated phases. In this case the results are significantly less accurate and somewhat puzzling: in particular it is not clear whether the transition is (weakly) first-order or second-order and, if this is the case, to which universality class it belongs.

Finally, we can point out another valuable use of our expansions as a guide for possibly more detailed MC investigations of models in the classes i) and ii), which might focus on specific points of the parameter space. Even more simply, our expansions can also serve as a realistic test-ground for techniques of analysis and re-summation of multivariate series. If nothing else, our calculations provide, for a variety of models, an initial set of HT reference data large enough to be a stringent constraint in the validation of future series extensions.

For completeness and in order to put our work into perspective, it is convenient to list the main existing HT results for the systems i) and ii) and to mention a few studies related to the subject of this paper, but using different techniques.

The earliest bivariate HT series investigation25 of the LP in the $N$-vector model with $nn$ and uniaxial $nnn$ interactions, was mainly devoted to the $N = 1$ case (namely the spin-1/2 Ising model). In three dimensions, series of order 8, 6 and 5 were derived for $N = 1, 2$ and 3, respectively. However, only the Ising HT series were considered25 by the authors long enough to yield sufficiently reliable numerical estimates of the location and the exponents of the LP. Both in two and three dimensions, the $N = 1$ series were subsequently extended25,30,31 through order 11 for the $J_1 - J_2$ interaction, for the 1-axial and for the $d$-axial interactions. Soon later, series for the susceptibility through the twelfth order were computed and analyzed32 for uniaxial models on the simple-cubic and the face-centered-cubic lattices. More recently, in two dimensions for the square-lattice Ising model, the susceptibility expansion was pushed39 through the thirteenth order for the $J_1 - J_2$ and the 2-axial interactions. These have been until now the longest bivariate series derived for systems with $nn$ and $nnn$ interactions.

For the $N \geq 2$ models, on the other hand, there has been no further progress in the HT calculations for the last three decades since the early sixth-order results25 in three dimensions. The only exception to this lack of activity was a study of the 2-axial $N$-vector model (with isotropic $nn$ and $nnn$ interactions on the square lattice), in which the bivariate HT series expansion coefficients were computed and tabulated through the fifth-order40, for general values of $N$. Interest into this model, which constitutes the “Symanzik improved”23 square-lattice formulation of the $O(N)$-symmetric non-linear $\sigma$-model in two-dimensional Euclidean field theory, came however from quantum field theorists. In particular, these HT expansions were derived as a means to infer the weak-coupling (i.e. LT) properties of the “improved” non-linear $\sigma$-model for $N \geq 3$.

A variety of MC investigations of models with $nnn$ interactions can also be found in the literature: most of them are concerned with the $N = 1$ case6,30,32,41,42,43,44,45, and some, more directly related to our work, with the $N = 2$ case. In particular, the uniaxial XY model in three dimensions was simulated in Refs.[46,47], its phase diagram was sketched out and the location of the LP was estimated along with the exponents of the susceptibility and the magnetization. Later investigations48,49 were devoted also to the $J_1 - J_2$ XY model in two dimensions. These studies were generally limited to only a few points in the interaction-
Before a systematic renormalization group approach could be extended to cover also the class of systems studied here, non-trivial technical difficulties, due to the anisotropy of the scale invariance in the critical behavior at LP’s, had to be solved. In particular, while the lowest order computation of all critical exponents by the $\epsilon$-expansion around the LP upper critical dimension $d_u(m)$ (with $\epsilon = d_u(m) - d$), as well as some $O(\epsilon^2)$ results, go back to three decades ago\(^8\), the extension through second order has been completed\(^50,51\) only recently. It is encouraging that the $O(\epsilon^2)$ corrections are small and decrease with increasing $N$, so that a simple truncation to order $\epsilon^2$ of the exponent expansions might already lead to reasonable approximations. Of course, further work is still needed before an accuracy comparable to that established for the usual critical points can be attained.

Results consistent with the $O(\epsilon^2)$ calculations for the exponents of the Ising 1–axial model in three dimensions have also been obtained\(^52\) from a truncation of the exact renormalization group equation. Renormalization group discussions of the ANNNXY model have been given in Refs.\(^53,54\).

There has been recent progress\(^55\) also in the calculation of the leading non-trivial corrections to the large $N$ limit\(^56\) for some exponents.

The layout of the paper is the following: In Sect. II the quantities for which we have computed HT expansions are defined in detail, and related to the main critical parameters in particular to the exponents of the uniaxial LP. The Sect. III is devoted to a discussion of the numerical analysis of the series. In the Appendix, we briefly describe the non-graphical algorithm used to compute the HT expansions and the checks passed by our series data.

III. THE HIGH-TEMPERATURE EXPANSIONS

In zero field and for any dimension $d$, for all models of the classes i) and ii) defined on bipartite lattices, the free energy is an even function of $J_1$ and therefore we can restrict our analyses to the case $J_1 > 0$ (ferromagnetic nn interaction).

In general, for $d > 1$ these models exhibit three main phases: a HT paramagnetic ($P$) phase, a LT uniformly-ordered ferromagnetic ($F$) phase and a family of LT ordered modulated ($M$) phases. For $d > 1$, a non-trivial transition line $K_{1c}(R)$ ($K_{1c}(R')$) separates the HT $P$-phase from the LT phases, whereas for $d = 1$, one has simply $K_{1c}(R) = \infty$. For $d > d_l(m)$, the critical line $K_{1c}(R)$ is divided into two branches by a LP, a triple point located at a non-zero value $K_{1c}(R_{LP})$ and separating the $P-F$-transition line from the $P-M$ line.

For $T = 0$, the spin ordering can be determined simply by minimizing the energy. The ferromagnetic ground state is energetically favored over the modulated phase(s) only for $R$ greater than some critical value. In the three-dimensional uniaxial case under study, the ground state is made of ferromagnetic layers orthogonal to the $z$-axis, with the relative orientation of the successive layers determined by the value of $R$.

It is clear that, except in the $d = 1$ case, in which the LT region is simply shrunk to the border of the paramagnetic region, the zero-field HT expansions are unsuited to yield much more than hints on the LT structure of the phase diagram and therefore, for the purpose of investigating the LT phases, they have to be replaced by other methods.

For all models of the classes i) and ii), we have derived the bivariate expansion of the
spin-spin correlation-function,
\[ C(\vec{0}, \vec{x}; K_1, R) = \langle \vec{\nu}(\vec{0}) \cdot \vec{\nu}(\vec{x}) \rangle, \]  
for all values of \( \vec{x} \) for which non-vanishing coefficients exist within the maximum order of expansion.

The appropriate quantities to be studied in order to locate the P-F branch of the critical line are the ordinary susceptibility
\[ \chi(K_1, R) = 1 + \sum_{\vec{x} \neq 0} \langle \vec{\nu}(\vec{0}) \cdot \vec{\nu}(\vec{x}) \rangle \]  
and the \( l \)-th order spherical moments of the correlation function
\[ m^{(l)}(K_1, R) = \sum_{\vec{x}} |\vec{x}|^l \langle \vec{\nu}(\vec{0}) \cdot \vec{\nu}(\vec{x}) \rangle. \]  

In terms of \( m^{(2)}(K_1, R) \) and \( \chi(K_1, R) \), we can construct the correlation length
\[ \xi^2(K_1, R) = m^{(2)}(K_1, R)/2d\chi(K_1, R) \]  

When studying a \( m \)-axial model with \( m < d \) and therefore with anisotropic interactions, it is convenient to break the \( d \)-dimensional lattice vectors \( \vec{x} \) as \( \vec{x} = (\vec{x}_\parallel, \vec{x}_\perp) \), where \( \vec{x}_\parallel \) and \( \vec{x}_\perp \) denote the \( m \)-dimensional and the \( (d-m) \)-dimensional components of \( \vec{x} \), respectively parallel and perpendicular to the directions of the \( nnn \) interaction.

In order to study the properties of the LP and to locate the P-M transition from the paramagnetic to the LT modulated phase it is necessary to study also the structure function with respect to \( \vec{q}_\parallel \)
\[ \chi(\vec{q}_\parallel; K_1, R) = 1 + \sum_{\vec{x} \neq 0} e^{i\vec{q}_\parallel \cdot \vec{x}} \langle \vec{\nu}(\vec{0}) \cdot \vec{\nu}(\vec{x}) \rangle \]  
and to \( \vec{q}_\perp \)
\[ \chi(\vec{q}_\perp; K_1, R) = 1 + \sum_{\vec{x} \neq 0} e^{i\vec{q}_\perp \cdot \vec{x}} \langle \vec{\nu}(\vec{0}) \cdot \vec{\nu}(\vec{x}) \rangle. \]  

In a vicinity of the LP, the scaling behavior of the two-spin correlation function becomes strongly anisotropic. In particular, the asymptotic behavior for large separation of spins joined by a vector whose components lie entirely in the \( m \)-dimensional \( \vec{x}_\parallel \) subspace, differs from the behavior in the case in which the spins are joined by a vector in the \( (d-m) \)-dimensional \( \vec{x}_\perp \) subspace. It is then necessary to replace each one of the usual correlation exponents \( \eta \) and \( \nu \) by a pair of exponents associated to the two subspaces. In the first case, the parallel correlation-exponent is usually denoted by \( \eta_\parallel \) (or less frequently, but more suggestively by \( \eta_{\parallel} \)), in the second case the transverse correlation-exponent is denoted by \( \eta_\perp \) (or by \( \eta_{\perp} \)). Correspondingly, in different directions two distinct correlation lengths \( \xi_\parallel \) and \( \xi_\perp \), are observed which diverge with different exponents \( \nu_\parallel \) and \( \nu_\perp \), respectively. These exponents are related to the susceptibility exponent \( \gamma_\parallel \) at the LP, by the “anisotropic scaling laws”
\[ \gamma_\parallel = (2 - \eta_\perp)\nu_\perp = (4 - \eta_\parallel)\nu_\parallel. \]
Moreover a generalized hyperscaling law is expected to hold:

\[ 2 - \alpha_l = m \nu_\parallel + (d - m) \nu_\perp. \]  

(10)

The other scaling relations: \( \alpha_l + 2\beta_l + \gamma_l = 2 \) and \( \gamma_l = \beta_l(\delta_l - 1) \) remain unchanged. We can thus conclude that three independent exponents are requested to characterize the uniaxial LP.

When \( d > d_u(m) = 4 + m/2 \), and \( m = 1 \), the critical exponents assume the \( N \)-independent mean-field values reported in Table I.

In order to estimate the additional critical exponents characterizing a LP, we have also computed the \( l \)-th order “parallel moments” of the correlation function

\[ m_l^{(l)}(K_1, R) = \sum_{\vec{x}} |\vec{x}_\parallel|^l < \vec{v}(0) \cdot \vec{v}(\vec{x}) >, \]  

(11)

and the \( l \)-th order “perpendicular moments”

\[ m_l^{(l)}(K_1, R) = \sum_{\vec{x}} |\vec{x}_\perp|^l < \vec{v}(0) \cdot \vec{v}(\vec{x}) >. \]  

(12)

Near the LP, the correlation length \( \xi^2_\parallel(K_1, R) \) in a direction within the \( m \)-dimensional subspace of the \( nnn \) interaction is then expressed in terms of these quantities by

\[ \xi^2_\parallel(K_1, R_{LP}) = m^{(2)}_\parallel(K_1, R_{LP})/2m\chi(0; K_1, R_{LP}) \sim \tau(R_{LP})^{-2\nu_\parallel} \]  

(13)

and analogously, the correlation length \( \xi^2_\perp(K_1, R) \) in a direction orthogonal to the \( nnn \) interaction by

\[ \xi^2_\perp(K_1, R_{LP}) = m^{(2)}_\perp(K_1, R_{LP})/2(d - m)\chi(0; K_1, R_{LP}) \sim \tau(R_{LP})^{-2\nu_\perp} \]  

(14)

with \( \tau(R) = T/T_c(R) - 1 \). Defining, in analogy with \( \tau(R_{LP}) \), the reduced competition ratio \( \rho_{LP} = R/R_{LP} - 1 \), a crossover exponent \( \phi \) can be introduced to characterize the behavior of the reduced critical temperature \( \tau_{LP} = T_c(R)/T_c(R_{LP}) - 1 \) as the LP is approached along the critical line: \( \tau_{LP} \sim |\rho_{LP}|^{1/\phi} \). Beside the above exponents, a related one: \( \beta_q = \nu_\parallel/\phi \) is associated to the LP. It describes the behavior of the magnitude of the modulation vector \( \vec{q} \) as the LP is approached along the branch of the critical line separating the disordered and the modulated ordered phases: \( |\vec{q}|^2 \sim \rho_{LP}^{2\beta_q} \).

IV. THE THREE-DIMENSIONAL UNIAXIAL (ANNNXY) MODEL

A. Universality along the \( P-F \) branch of the critical line

For \( R \) in the range \(-1/4 < R < \infty \), the ground state of the system is ferromagnetic and the uniform ferromagnetic ordering persists at \( T > 0 \) up to some inverse temperature \( K_{1c}(R) \), at which a second-order phase transition, expected to belong to the universality class of the three-dimensional XY model, occurs between the LT phase and the HT paramagnetic phase.

In this subsection we shall mainly discuss the numerical evidence obtained from the analysis of our HT series that, in the ferromagnetic range of \( R \), this transition actually
belongs to the XY universality class. We shall then argue that, if this is the case, the parameter $R$ can be exploited to determine very accurate values of the critical exponents for the XY universality class.

For each value of $R$, we can locate the transition by analyzing the HT expansion of the ordinary susceptibility $\chi(K_1, R)$, whose coefficients show generally a smooth dependence on the order of expansion and a fast approach to their asymptotic forms, and thus are well suited to numerical study.

The critical behavior of the susceptibility as $\tau(R) \to 0^+$ is expected to be

$$\chi(K_1, R) = A_\chi^+(R) \tau(R)^{-\gamma(R)} \left(1 + a_\chi^+(R) \tau(R)^{\omega(R)} + O(\tau(R))\right)$$

(15)

where $A_\chi^+(R)$ is the critical amplitude of the susceptibility, and $a_\chi^+(R)$ is the leading correction-to-scaling amplitude. We have denoted $\gamma(R)$ and $\omega(R)$ as a priori $R$-dependent, although we shall finally argue that, as expected, they are universal with respect to $R$, namely independent of $R$.

The critical behavior of the second-moment correlation length may analogously be characterized as

$$\xi^2(K_1, R) = A_{\xi^2}^+(R) \tau(R)^{-2\nu(R)} \left(1 + a_{\xi^2}^+(R) \tau(R)^{\omega(R)} + O(\tau(R))\right).$$

(16)

We shall re-sum the susceptibility series by inhomogeneous second-order DAs in the variable $K_1$ at fixed $R$. In this and in the analyses that follow, we have used a set of quasi-diagonal DAs chosen as the approximants $[k,l,m;n]$ with $14 \leq k + l + m + n \leq 16$, namely those using not less than 17 series coefficients. We have taken $|k-l|, |l-m|, |k-m| < 3$ with $k,l,m > 3$, while $1 \leq n \leq 4$. We have however always made sure that our numerical estimates depend only weakly on this choice. The results for the critical line obtained in this way (for $R_{LP} \lesssim R \lesssim 2$) are reported in Fig. 11. Notice that we have preferred to plot vs $R$ the quantity $T_c(R)/2 = 1/2 K_{1c}(R)$ rather than $K_{1c}(R)$ itself, in order to make our figure immediately comparable with the figure, covering a smaller range of $R$, which appears in the MC study of Ref. [46]. On the scale of Fig. 11 the three data points ($R = 0.1, T_c(R)/2 = 2.17(2)$), ($R = -0.25, T_c(R)/2 = 1.83(2)$) and ($R = -0.26, T_c(R)/2 = 1.82(2)$) obtained in the MC study, are hardly distinguishable from our curve. The corresponding values determined by our series are: ($R = 0.1, T_c(R)/2 = 2.2017(2)$), ($R = -0.25, T_c(R)/2 = 1.830(1)$) and ($R = -0.26, T_c(R)/2 = 1.809(1)$). Our result at $R = 0$. compares well with the estimate ($R = 0.1, T_c(R)/2 = 2.20172(15)$), obtained by 21th-order HT expansions. Notice also that the spreads $\delta K_{1c}(R)$ of our DA estimates of the critical temperatures, which are smaller than those of the MC study by one order of magnitude, are invisible on the scale of the figure. For convenience, we have listed in Table II a few numerical values of $K_{1c}(R)$.

It should be stressed that it is generally difficult to assess very accurately the real uncertainties of the results in this kind of analysis mainly because, due to the finite (and in our case still moderate) length of the series, the sequences of DA estimates may retain residual trends which call for further extrapolation, particularly so for $R \gtrsim 1$. Whenever possible, one should then try to infer the size of the uncertainties also from a comparison with the results of approximation procedures alternative to the direct DA calculation, and thus presumably having different convergence rates and different mechanisms of error build-up. In our case, we shall eventually argue that the spread of the DA estimates of the critical temperature, already at these orders of HT expansion, are reasonable approximations of the uncertainties, at least for positive and not too large $R$. 

9
Let us then consider an example of an alternative approach to the determination of \(K_{1c}(R)\). If the critical singularity is the nearest singularity, we can determine it also by evaluating the limit of the sequence of estimators \((K_{1c}(R))_n\) of \(K_{1c}(R)\) defined by the modified-ratio prescription\(^{28,35}\):

\[
(K_{1c}(R))_n = \left(\frac{c_{n-2}c_{n-3}}{c_{n}c_{n-1}}\right)^{1/4} \exp\left[\frac{s_n + s_{n-2}}{2s_n(s_n - s_{n-2})}\right]
\]  \(17\)

where

\[
s_n = \left(\ln\left(\frac{c_{n-2}}{c_{n}c_{n-4}}\right)^{-1} + \ln\left(\frac{c_{n-3}}{c_{n-1}c_{n-5}}\right)^{-1}\right)/2
\]  \(18\)

and \(c_n(R)\) are the HT expansion coefficients of the susceptibility.

This prescription has the important advantage of bringing information not only about \(K_{1c}(R)\), but also on the leading correction-to-scaling amplitude \(a_\chi^+(R)\), defined by eq.\(^{15}\), a quantity which in general rules the convergence properties of any approximation method in the critical region. Indeed, we have observed\(^{26}\) that the modified-ratio sequence has the simple asymptotic behavior for large order \(n\)

\[
(K_{1c}(R))_n = K_{1c}(R) \left(1 - \frac{C(\gamma, \omega)a_\chi^+(R)}{n^{1+\omega}} + O(1/n^2)\right)
\]  \(19\)

where \(C(\gamma, \omega)\) is some known positive function of \(\gamma\) and \(\omega\).

In order to use effectively the modified-ratio method, we shall now assume that the exponent \(\omega = \omega(R)\) of the leading correction to scaling is independent of \(R\), and takes the value\(^{58}\) \(\omega \approx 0.52\) (an assumption which was not necessary to make in the DA method discussion). Then by fitting the sequence \((K_{1c}(R))_n\) to the simple form \(b_1(R) - b_2(R)/n^{1+\omega}\), we can estimate the amplitude \(a_\chi^+(R)\) from the value of the parameter \(b_2(R)\). Although rather long and smooth series are usually necessary\(^{26}\) to obtain accurate estimates by this method, we can observe a complete consistency between the estimates of \(K_{1c}(R)\) from the DAs and the values of \(b_1(R)\) obtained by the fit (within a small multiple of their spreads, for positive and not too large \(R\)), so that the results cannot be distinguished from those reported in Fig.1. This fact also gives support to our simple fit procedure for determining \(b_2(R)\) and, at the same time, it suggests that the spread of the DA estimates of the critical temperatures might be taken as a sound measure of their real uncertainties. In order to illustrate our fit procedure for determining \(b_2(R)\), in Fig.2 we have plotted vs \(x = 1/n^{1+\omega}\) the sequence of modified ratios \((K_{1c}(R))_n\) normalized to their extrapolated values \(b_1(R)\), for a few fixed values of \(R\), chosen in a vicinity of \(R_M\). Let us add that only for \(R \gtrsim 0\) the sequences \((K_{1c}(R))_n\) are sufficiently smooth that these rough, but sufficiently reliable, estimates of \(b_2(R)\) are feasible, while unfortunately for \(R < 0\) the modified-ratio sequences develop strong oscillations and a straightforward two-parameter fit cannot work. The important observation is now that the function \(b_2(R)\) vanishes at \(R = R_M \approx 0.28(3)\) and therefore its absolute value is minimum at this point. From our estimates of \(b_2(R)\), we can infer the sign and size of the deviations from the exact values which should be expected for the central DA estimates of \(K_{1c}(R)\) and of the exponents, as \(R\) varies. More precisely, we have to expect\(^{50}\) that, in the range \(R > R_M\), where \(b_2(R)\) and therefore \(a_\chi^+(R)\) are found to be positive, the critical inverse temperatures and the critical exponents will be underestimated by our analyses, while the opposite will be observed for \(R < R_M\). This is clear from eq.\(^{19}\) as far as the critical inverse temperatures are concerned. In order to reach the same conclusion for the
exponents, one may either use an asymptotic formula\textsuperscript{26} analogous to eq.\textsuperscript{19} or consider that in approximate calculations some effective exponent\textsuperscript{26} is generally evaluated, for example:
\[ \gamma_{\text{eff}}(\bar{\tau}) = -\frac{d\log(\chi)}{d\log(\bar{\tau})} \simeq \gamma - \omega a_\chi^{+} \bar{\tau}^\omega \] with \( \bar{\tau} \) small, but nonzero. In order to relate these remarks to the behavior of \( b_3(R) \), the absolute value of \( b_3(R) \), obtained from a fit of the four highest-order estimators \((K_{1c}(R))_n\) in the modified-ratio sequence, is very schematically plotted vs \( R \), together with the exponent estimates, in Figure\textsuperscript{3} and in some of the following figures. All previous considerations also apply to the study of the HT expansion of \( \xi^2(K_1, R) \).

In Figure\textsuperscript{4} the critical exponents \( \gamma(R) \) of the susceptibility and \( \nu_\perp(R) \) of the transverse correlation-length (notice that \( \nu_{\parallel}(R) \) and \( \nu_{\parallel}(R) \) coincide with \( \nu(R) \) for \( R \gtrsim 0 \)) are plotted as functions of \( R \) along the P-F branch of the critical line. They have been computed both using second-order DAs biased with the critical singularity \( K_{1c}(R) \) and, alternatively, also by the method of “critical-point renormalization”\textsuperscript{60}. The latter method consists in analyzing the term-by-term divided series \( W(x, R) = \sum_d d\_n(R)/c\_n(R)x^d \), where \( d\_n(R) \) are the expansion coefficients of \( \chi(K_1, R) \) (or of \( \xi^2(K_1, R)/K_1^2 \)) and \( c\_n(R) \) are the coefficients of \( \chi(K_1, R) \) (or of \( \xi^2(K_1, R)/K_1 \)). It can be shown that, if the nearest singularity is the critical point, then \( W(x, R) \) is singular at \( x = 1 \) with an exponent \(-\left(1 + \gamma(R)\right)\) (resp.\(-\left(1 + 2\nu(R)\right)\)), which can be estimated by forming DAs of \( W(x, R) \) biased to be singular at \( x = 1 \). This alternative determination of the exponents is of particular interest in the ranges of values of \( R \) in which the accuracy of the available estimates of \( K_{1c}(R) \) might be insufficient to obtain good temperature-biased estimates or where the convergence of the DAs is slow. It is not surprising that in a neighborhood of \( R_M \) (where the amplitude of the leading correction to scaling is vanishing), this method and the direct analysis of the susceptibility (or of the correlation length) by temperature-biased DAs yield essentially the same exponent estimates, while elsewhere they show some small difference. In Fig.\textsuperscript{3} the results of both approximations are plotted vs \( R \) and compared with a recent high accuracy determination\textsuperscript{38} \( \gamma = 1.3178(2) \) and \( \nu = 0.67155(27) \) of the exponents \( \gamma \) and \( \nu \) for the XY universality class. Our two approximations for \( \gamma(R) \) and \( \nu(R) \) show a similar behavior: for \( R > R_M \) both lead to estimates slightly smaller than the data chosen for comparison, while the opposite happens for \( R < R_M \). This is precisely what can be anticipated from our determination of the leading correction-to-scaling amplitude. Overall, as shown in Figure\textsuperscript{3} for \( 0 \lesssim R \lesssim 1 \), the central values of our estimates of the critical exponents deviate from the estimates at \( R = R_M \) by less than 0.5%, while in the wider range \( 0 \lesssim R \lesssim 1.5 \) the deviations do not exceed 1%, thus indicating that our approximate results have a very weak dependence on \( R \), to within a fair accuracy. Even more accurate results are obtained computing, for example by simplified\textsuperscript{61} DAs, (biased with \( K_{1c}(R) \) and with the correction-to-scaling exponent \( \omega \)), the ratio of the log-derivatives of the quantities \( m^{(2)}_\perp(K_1, R)/K_1 \) and \( \chi(K_1, R) \), which yields the ratio \( \nu_\perp(R)/\gamma(R) \). As it is also shown in Fig\textsuperscript{3} the estimates so obtained for this ratio appear to be independent of \( R \) to within 0.1% along the whole interval \( 0 \lesssim R \lesssim 1.5 \), in which they remain quite near to the ratio of the data\textsuperscript{38} chosen for comparison. Of course, this particularly favorable result is simply due to the fact that the relative deviations of \( \gamma(R) \) and \( \nu_\perp(R) \), with respect to their values at \( R_M \), keep the same sign and a similar size as \( R \) varies.

A blow-up view of part of these results is presented in Fig\textsuperscript{4} where we have plotted our temperature-biased DA estimates of the exponents \( \gamma(R) \), \( \nu_\perp(R) \) and of their ratio, after normalizing them to the corresponding comparison\textsuperscript{38} values.

It is amusing to remark that, for positive and not too large values of \( R \), our rough determination of the behavior of \( a_\chi(R) \) also suggests a simple prescription to improve the
estimates of the exponents by temperature-biased DAs. We have simply to correct for the expected errors in the bias values of $K_{1c}(R)$, computing the critical exponents by DAs biased with $K_{1c}(R) + \delta K_{1c}(R)/2$ when $R > R_M + 0.03$, or with $K_{1c}(R) - \delta K_{1c}(R)/2$ when $R < R_M - 0.03$. We have shown in Fig[5] that this quite naive adjustment of the standard biasing procedure to account for the sign and size of $\delta K$ improves visibly the universality of the exponents with respect to $R$. At the same time, this result gives further support to our conjecture that the spread $\delta K_{1c}(R)$ of the DA estimates of $K_{1c}(R)$ is a sound approximation of their uncertainty, provided that $R$ is positive and not too large.

We have also studied other indicators of universality, such as, for example, the values at the critical point $K_{1c}(R)$ of the correlation-moment ratios

$$Q(p, q; r, s; R) = \frac{m^{(p)}(K_1, R)m^{(q)}(K_1, R)}{m^{(r)}(K_1, R)m^{(s)}(K_1, R)}$$

with $p + q = r + s$. As expected, they show an approximate independence on $R$ for $R > 0$. This is shown in Fig[6] where we have plotted vs $R$ a few ratios $Q(p, q; r, s; R)$ evaluated at the critical point and normalized to their value $Q(p, q; r, s; R_M)$ at $R_M$. Our estimates refer to the cases in which $(q = p = 1/2; r = 1/4, s = 3/4)$, or $(q = 1/2, p = 1/4; r = 0, s = 3/4)$ or $(q = p = 1/2; r = 0, s = 1)$.

As long as $R$ is positive and not too large, we can conclude that all these results consistenly and rather convincingly indicate that, along the $P-F$ branch of the critical line, the small violations of the exponent universality with respect to $R$, shown by our numerical computations, are only apparent and can be entirely ascribed to the slow convergence of approximation procedures still unable, at the present orders of expansion, to account fully for the presence of corrections to scaling.

These evidences of universality with respect to $R$ justify the technique[35,36] that we can adopt in order to improve the accuracy in the determination of the exponents for the XY universality class. We can observe that, as $R$ varies in the ferromagnetic range, we have an $R$-dependent family of models all of which can be assumed to belong to the XY universality class, so that they share the same critical exponents, while they have generally different $R$-dependent (namely non-universal) amplitudes of the corrections to scaling. Therefore, we expect that the best approximations for the universal quantities will be achieved from the study of the model with $R = R_M$, because $a^{+}_\chi(R_M)$ vanishes. For this particular model in the family also the other leading correction amplitudes of interest, for example $a^{+}_{\xi_2}(R)$, must vanish at $R_M$, since the correction-amplitude ratios such as $a^{+}_\chi(R)/a^{+}_{\xi_2}(R)$ are universal.

These arguments support our belief that our exponent estimates $\gamma(R_M) = 1.3177(5)$, $\nu(R_M) = 0.6726(8)$ and $\nu(R_M)/\gamma(R_M) = 0.5100(1)$ should be rated as the best possible determinations of the susceptibility and correlation-length exponents in the XY universality class, that one can extract, at the present expansion order, from our $R$-dependent family of HT series.

The high-precision estimates[35] of the XY universality class exponents that we have compared to our results in Fig[3], were also obtained using a similar improvement procedure in the case of a different family of $nm$-interaction models for which series of order 23 are known. Our best estimate of the susceptibility exponent agrees well with the corresponding result cited for comparison, although the uncertainty of our result is sizably larger, due to the still moderate length of our bivariate series. On the other hand, the central value of our best estimate for the exponent $\nu$ is somewhat larger than (while the estimate $\nu = 0.6720(4)$
obtained from those of \( \gamma \) and of the ratio \( \nu/\gamma \) is much closer to the corresponding comparison value. Our direct estimate of \( \nu \) is closer to the older MC result\[62,67\] \( \nu = 0.6723(3) \) and to the result \( \nu = 0.6717(3) \) of the simulation of Refs.\[63,64\]. It is, however, much larger than the value \( \nu = 0.6709(1) \) obtained, by using the hyperscaling relation \( 2 - \alpha = d\nu \), from the recent high-accuracy measure \( \alpha = 0.0127(3) \) of the \(^4\)He specific heat in a micro-gravity experiment\[65\].

In Ref.\[63\] recent determinations of \( \nu \) with increasing accuracy have been summarized into a useful diagram showing that the central estimates from the most recent MC simulations and HT series analyses are, in general, significantly larger than those obtained both from the renormalization group and from the cited experimental measure. This is an interesting remark which calls, at least, for a more accurate reassessment of the uncertainties of the results in the literature. As far as our HT approach is concerned, we can reasonably expect that an extension of the bivariate expansions by only a couple of orders would significantly reduce the uncertainties of our best estimates of the exponents, particularly so for the direct estimate of \( \nu \). Presently, however, it might be less difficult to give further support to our arguments and make them sharper by using our series results as a guide for a high-precision MC simulation of the ANNNXY model at \( R = R_M \).

Finally we must add that, unfortunately, our series for the specific heat, which is a very weakly singular quantity, seems to be still insufficiently long to yield an evaluation of comparable accuracy for the exponent \( \alpha(R) \). We can only infer that on the \( P-F \) line, \( \alpha(R) \simeq -0.01(2) \), as expected. This result is completely compatible with the bounds \( -0.0202 < \alpha < -0.0124 \) obtained introducing into the hyperscaling relation the extremal values of the range of estimates of \( \nu \) reported in the recent literature.

We can conclude our study of the critical behavior along the \( P-F \) line remarking that from a study of \( T_c(R) \) in a vicinity of \( T_{LP} \), we can estimate \( \phi = 1.00(4) \), since it appears that the curve \( T_c = T_c(R) \) changes from concave to convex in a small vicinity of \( T(R_{LP}) \).

**B. The Lifshitz point and the \( P-M \) branch of the critical line**

In the mean-field approximation \( R_{LP} = -1/4 \), but our HT calculation shifts this value by \( \simeq 10\% \) to the modulated side of the phase diagram. For \( R_{LP} < R \lesssim 0 \), the critical exponents crossover from the value of the XY universality class to the LP critical behavior. In this range of \( R \), the amplitudes \( a_\chi^+(R) \) and \( a_\xi^+(R) \) appearing in eqs.\[15\] and \[16\] lose their leading role, because also higher order correction amplitudes become important, the convergence of our series slows down and they appear inadequate to exhibit the universality with respect to \( R \) of the exponents and their expected discontinuous change to the values of the LP universality class at \( R = R_{LP} \). Thus, of course, in the crossover region, also the spreads of our estimates will grossly underestimate the real errors.

Let us now recall that the eq. \( m_\parallel^(2)(K_1, R) = 0 \) implicitly defines in the \( R - T \) plane the so-called disorder line\[7\], which, within the paramagnetic phase, divides a region with monotonically (exponentially) decaying correlations along the direction parallel to the \( nnn \) interaction from a region with oscillating, but still exponentially damped correlations. The equation defining the disorder line can be solved iteratively with respect to \( R \) to form the single-variable series \( R_{dis} = R_{dis}(T) \), which finally is re-summed by DAs. The plot of the disorder line obtained from this series is drawn as an almost vertical dashed line in Figure \[1\] It may be of interest to show how accurately the spin-spin correlations can be computed
at HT and therefore we have displayed in Fig[7] the qualitative difference in their behavior as functions of the distance of the spins along the $z$-direction, on the two sides of the disorder line. Using our knowledge of the spin-spin correlations, we can also show that the LT modulated order already begins to build up in the nearly critical HT phase. This is suggested by Fig[8] where we have plotted vs $z$ the values of the energy, the $nn$ and the $nnn$ spin correlations along the $z$-axis, calculated just above the boundary of the paramagnetic phase, precisely at $T = 1.1T_c(R)$. We can observe that the energy reaches a maximum near $R_{LP}$, where the disorder is higher and that the $nn$ spins are positively correlated on the whole range of $R$ (albeit not too strongly since $T$ is high). On the other hand the $nnn$ spins tend to be more correlated than the $nn$ spins for $R \gtrsim 1.2$, while as $R$ is lowered, this correlation decays to become negative when $R \lesssim R_{LP}$.

In order to locate the LP on the boundary of the paramagnetic phase, we have to recall[25,32] that for small $q_z$

$$
\chi(0, K_1, R)/\chi(q_z, K_1, R) = 1 + q_z^2 \frac{m^{(2)}(K_1, R)}{2\chi(K_1, R)} + q_z^4 \left( \frac{m^{(2)}(K_1, R)^2}{4\chi(K_1, R)^2} - \frac{m^{(4)}(K_1, R)}{24\chi(K_1, R)} \right) + \ldots (21)
$$

showing that the minimum at $q_z = 0$, which characterizes $\chi(0, K_1, R)/\chi(q_z, K_1, R)$ at fixed $K_1$, when $R$ is in the ferromagnetic range, changes to a local maximum as $R \to R_{dis}(K_1)$ where the second-order parallel moment $m^{(2)}(K_1, R) = 0$. Thus the LP is found at the intersection of the $P$-$F$ branch of the critical line with the disorder line. Following this procedure we are led to the estimate $(R_{LP} = -0.2733(6), T(R_{LP}) = 1.778(2))$ of the intersection point between the critical locus and the disorder line. The value of $R_{LP}$ obtained in this way is consistent with that obtained minimizing $\chi(0, K_1, R)/\chi(q_z, K_1, R)$ with respect to $q_z^2$ as $R - R_{LP} \to 0^-$ and $K_1 \to K_1(R)$. Indeed, for small $q_z^2$, we obtain from eq.(21) that the position of the minimum $q_z^2$ vs $R$ is given by

$$
q_z^2 \approx \frac{6m^{(2)}(K_1, R)\chi(K_1, R)}{m^{(4)}(K_1, R)\chi(K_1, R) - 6m^{(2)}(K_1, R)^2} \quad (22)
$$

evaluated at the critical point $K_{1c} = K_{1c}(R)$ for $R \lesssim R_{LP}$. By re-summing the series expansion of $q_z^2$, we can determine $R_{LP}$, also as the value of $R$ at which $q_z^2 = 0$.

For $R \lesssim 0$, in the crossover region, Figs[3] and [9] show a steep rise of our exponent estimates near the LP and past it, followed by a somewhat slower decay extending through $R \simeq -0.8$. A completely similar behavior of the exponent $\gamma(R)$ near the LP was noted in a HT study[32] of the 3d ANNNI model. In this study, we should then assume that the values of the exponents at the LP are not strongly affected by the crossover and also be aware that they are rather sensitive to the location of the LP. Using the critical-point renormalization method, we can estimate $\gamma_l = 1.55(1)$, while the biased DAs suggest $\gamma_l = 1.52(1)$, as shown in Fig[8]. We shall take a weighted average of these values as our final estimate of the exponent: $\gamma_l = 1.535 \pm 0.025 \pm 0.2|R_{LP} + 0.2733|$, including explicitly in our error a contribution from the uncertainty of $R_{LP}$. This result has a smaller uncertainty than but is completely compatible with the estimate $\gamma_l = 1.5(1)$ of the MC simulation of Ref.[47]. Notice that our estimates of $R_{LP}$ and $T(R_{LP})/2.$ differ by $\approx 5\%$ from the values $R_{LP} = -0.263(2)$ and $T_{LP}(R)/2. \simeq 1.82$, determined by the old (sixth-order) series[25] and used as an input in the MC[46,47] study. Our estimate of the exponent is also not far from the value $\gamma_l = 1.495$ obtained[50,55] simply by setting $\epsilon = d_\alpha(1) - d = 3/2$ in the two-loop $\epsilon$-expansion.
Starting with the HT expansions of $\xi^t_\perp(K_1, R)$, similar considerations yield the estimate $\nu_\perp = 0.805 \pm 0.015 \pm 0.1[R_{LP} + 0.2733]$. For this exponent, no MC results are available and our result can be compared only with the value $\nu_\perp = 0.757$ from the $\epsilon$-expansion.

The direct estimate of $\nu_\parallel$ from the analysis of $\xi_\parallel$ is notoriously difficult because, in the $P$ phase near the Lifshitz point, the competition between the $nn$ and the $nnn$ interaction reduces drastically the correlation length in the $z$ direction. In particular, in the $N = 1$ case, the determination of $\nu_\parallel$ has so far eluded even the most extensive MC simulation so far available. In the large $N$ limit (namely in the case of the uniaxial spherical model), in which very long HT expansions can be easily computed, it was observed that at least 35 orders are necessary to approximate the behavior of $\xi_\parallel$! Also in the $N = 2$ case under study, the length of our HT expansions, unfortunately, seems to be still insufficient. We can, however, try to estimate indirectly $\nu_\parallel$, either from a measure of the exponents $\beta_\parallel$ and $\phi$, taking advantage of the scaling law $\nu_\parallel = \beta_\parallel \phi$, or by determining the exponent $\alpha_l$ and then using the generalized hyperscaling law along with our previous estimate of $\nu_\perp$. As above remarked, the determination of the exponent $\alpha_l$ from our series is not yet accurate enough to be useful. It does suggest, however, that $\alpha_l = -0.02(2)$, which is compatible with the $\epsilon$-expansion estimate in Table I. If, quite conservatively, we simply assume that $\alpha_l$ is negative and $|\alpha_l| < 0.1$, we get from the hyperscaling law the rough bounds $0.36 < \nu_\parallel < 0.52$, which are consistent with the $O(\epsilon^2)$ value $\nu_\parallel \simeq 0.372$ reported in Table I. On the other hand, using the above reported estimate $\phi = 1.00(4)$ and the estimate $\beta_\parallel = 0.40(2)$ given below, we get the value $\nu_\parallel = 0.40(3)$. Plugging back this result into the hyperscaling law, we find the value $\alpha_l = -0.01(6)$ for the specific-heat exponent, which is also compatible with all above indicated estimates. The values of the remaining exponents can all be obtained from the scaling laws.

We can thus conclude that our HT determinations of the critical exponents at the LP are in most cases consistent, to within $\simeq 10\%$, with the $\epsilon$-expansion estimates.

In order to map out the branch of the critical line with $R < R_{LP}$, we have to analyze the wave-vector-dependent susceptibility $\chi(q_z, K_1, R)$. For $R < R_{LP}$ the critical point $K_{lc}(R)$ can be determined by locating the nearest positive singularity in $K_1$ of $\chi(q_z, K_1, R)$ with $q_z$ near the peak value $q^*_z = \bar{q}_z(K_1, R)$. The value of $K_{lc}(R)$ is taken to be the minimum with respect to $q_z$ of the singularity locus $K_1 = K_{1c}(q_z, R)$ of $\chi(q_z, K_1, R)$. Our results for the $P-M$ branch of the critical line, also drawn in Fig[1] complete the map of the boundary of the paramagnetic phase. In the same figure, we have schematically indicated a transition line, which separates the ferromagnetic and the modulated phases and joins the LP to the point $R = -1/4, T = 0$, where the ordering of the ground state changes from ferromagnetic to modulated. This line is also expected to be of second order, but is beyond the reach of our HT analysis. Our phase diagram agrees well with the cited results obtained supplementing a MC simulation with the sixth-order HT expansions of Ref. [25].

It must be noted that the uncertainties of the points of the $P-M$ branch of the critical line are sizably larger than those of the $P-F$ branch, making it more difficult to obtain precise temperature-biased estimates of the critical exponents. If, nevertheless, we insist in computing some rough estimate of the exponent $\gamma(R)$, it is encouraging to observe that the results obtained from temperature-biased DAs remain essentially consistent, over a wide range of values of $R$, with those computed by the critical-point renormalization method which is insensitive to the uncertainties of the critical temperatures. The results for $\gamma(R)$ obtained by these two methods are reported in Fig[9] For $R < -0.8$, on the left of the region of crossover from the value of $\gamma_l$, we observe that both sequences of estimates tend to stabilize.
at some value which is intermediate between those of the $O(2)$ and of the $O(3)$ universality classes. These puzzling results might deserve further confirmation by a MC study. If they are confirmed, the MC approach\textsuperscript{67} would also be best suited to investigate whether a possible (weak) first-order\textsuperscript{68} (rather than second-order) character of the $P-M$ transition might explain its features. This possibility was suggested by a renormalization group study of a Landau-Ginzburg effective four-component model of a biaxial $N = 2$ system\textsuperscript{53} which turned out to have only unstable fixed points at second order in the $\epsilon$-expansion.

The curve describing the peak value $\bar{q}_z$ of the modulation wave-number $q_z$ at $T = T_c(R)$ vs $R$, obtained from our analysis, is reported in Fig.10 and compared to the mean-field prediction $\bar{q}_z^{MF}(R) = \cos^{-1}(R_{LP}^{MF}/R)$ with $R_{LP}^{MF} = -1/4$. As pointed out in Ref.\textsuperscript{25}, also in the Ising case, at high temperature the peak of $\chi(q_z, K_1, R)$ occurs at $\bar{q}_z^{MF}(R)$ but, as the temperature decreases to $T_c(R)$, the peak moves to lower values of $q_z$ for $R \gtrsim -0.6$ or otherwise to slightly higher values. This is clearly shown in Fig.10. The largest deviations of our results from the mean-value approximation occur in a small vicinity of $R_{LP}$.

From the behavior of this curve near $R \simeq R_{LP}$, we have estimated the value $\beta_q = 0.40(2)$ used above.

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APPENDIX A: DERIVATION AND VALIDATION OF THE SERIES

We have used the algorithm\textsuperscript{69} of the Schwinger-Dyson equations(SDE) to compute the HT expansions for the $N$-vector spin models under study. When it was introduced, the SDE method could be profitably applied only to systems with $nn$ interactions\textsuperscript{70}, due to the severe limitations in the memory and speed of the computers available two decades ago. This method was repeatedly described in Refs.\textsuperscript{70,71}, and therefore it is sufficient to recall only that for the XY models described by the Hamiltonians (1) and (2), the SDE take a particularly simple and suggestive form. Indicating by $s = (\mathbf{x}_1, q_1; \mathbf{x}_2, q_2; ... \mathbf{x}_k, q_k)$ a set of site coordinates $\mathbf{x}_i$ and of integer nonzero quantities $q_i$ attached to them and such that $\sum_{i=1}^k q_i = 0$, the generic correlation function can be written as

$$< \phi(s) > = \frac{1}{Z} \int \Pi_x d\theta_x \phi(s) e^{-\beta H}$$

(A1)

where $\phi(s) = \exp[i \sum_{k} q_k \theta_{x_k}]$ and $\theta_x$ is the angle formed by the unit vector $\mathbf{v}(\mathbf{x})$ with a fixed direction. The SDE are:

$$< \phi(s) > = -\frac{K_1}{q_1} \sum_{\mu} (< \phi(s_{\mu}^+)) - < \phi(s_{\mu}^-)) > - \frac{K_2}{q_1} \sum_{\nu} (< \phi(s_{\nu}^+)) - < \phi(s_{\nu}^-)) >$$

(A2)
Here
\[ \phi(s^+_{\mu}) = \exp(i\theta_{x1}) \exp(-i\theta_{x1+a_\mu})\phi(s), \] (A3)

while
\[ \phi(s^-_{\mu}) = \exp(-i\theta_{x1}) \exp(i\theta_{x1+a_\mu})\phi(s). \] (A4)

Moreover
\[ \phi(s^+_{\nu}) = \exp(i\theta_{x1}) \exp(-i\theta_{x1+b_\nu})\phi(s), \] (A5)

and
\[ \phi(s^-_{\nu}) = \exp(-i\theta_{x1}) \exp(i\theta_{x1+b_\nu})\phi(s) \] (A6)

with \( \vec{x}_1 \) an arbitrary site in the set \( s \). In the first sum of eq. (A2), \( a_\mu \) is the lattice vector joining the site \( \vec{x}_1 \) to the \( nn \) sites, whereas in the second sum \( b_\nu \) denotes the vector joining the site \( \vec{x}_1 \) to the \( nnn \) sites in the case of the Hamiltonian eq. (1) (the vector joining the site \( \vec{x}_1 \) to the \( sn \) sites in the case of the Hamiltonian eq. (2)).

The computational complexity of the SDE method increases with the lattice dimensionality and, for a given dimensionality, with the effective coordination-number, i.e. as the number of interacting neighbors increases. Essentially the same difficulty is met with the evaluation of the embedding factors in the conventional graph approach, but our method has the advantage of using the SDE as recurrence relations among the correlation functions and of requiring only a straightforward iteration of these relations, which avoids altogether all combinatorial intricacies of the graph method. In the specific cases under study, due to the presence of the \( nnn \) interactions, this method is, by some orders of magnitude, more memory and CPU demanding than for the pure \( nn \) interactions, but otherwise not much more difficult. Thus for example, in the computationally most intensive case: that of the Hamiltonian of eq. (1) in 3d with 3 - axial interaction, the general SDE is a linear relationship among 25 \textit{a priori} different, correlation functions, while in the simpler \( nn \) interaction case in three-dimensions, the SDE involve only 13 correlation functions.

A carefully designed code for the Schwinger-Dyson equations can compute moderately long series using only a reasonable CPU time of an ordinary 32-bit single-core processor desktop PC. In particular, our codes can reproduce all previously existing series data in a negligible CPU time of the order of \( 10^{-3} \) sec. Due to the sensitive dependence of the computational load on the effective coordination number, the series that we could derive for the \( 1 - axial \) models are longer (and more fastly computed) than those for the \( d - axial \) models. In the case of the uniaxial model studied here, the expansion through order 17 was completed in approximately three weeks by a PC, while the order 18 was obtained by using a few nodes of a PC cluster for an equivalent single-processor CPU-time of approximately five months. Longer series might be obtained by a more extensive parallelization of our codes or, perhaps, by returning to the conventional graph methods, provided that the efficiency of the current graph-embedding algorithms can be drastically improved.

The comparison of the extended expansions with independent, sufficiently long and reliable previous results is always a necessary step in the validation of the codes and of the results for automated derivations. Generally, in our case, this was not satisfactorily feasible. In two dimensions, a comparison was possible only for the 2-axial model (1), for which a fifth-order expansion of the susceptibility was tabulated in Ref.[40] and in three-dimensions, only in the case of the 1-axial model, for which an expansion of the susceptibility was tabulated through sixth order in Ref.[25]. Our series agree with these results. Due to the lack of other published data and to the present unavailability of old short unpublished series for the 3-axial case in three dimensions, no further comparison with independent calculations.
was possible. Weaker (and obvious) tests, through all orders that we have computed, are feasible in the limiting cases in which one of the exchange interaction constants vanishes. For example, when $K_2 = 0$, the series for the $m$-axial models should reduce to those of the $nn$ interaction models on the same lattice. Therefore the series for the $1$-axial models should reduce to those of a $nn$ interaction model on the same lattice when $K_2 = 0$, and to those of a $nn$ model on a $1d$ lattice when $K_1 = 0$. Of course, our results pass also these tests, which however pin down only 2 out of the $l + 1$ coefficients of each order $l$. Our confidence in the correctness of the calculations, for which we have written two sets of largely independent codes, in Fortran and in C++, receives further support also from the stability of the numerical results under our many rewritings of both sets of codes to increase their efficiency, as well as from the smooth and consistent behavior of the quantities analyzed.

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FIG. 1: The phase diagram of the three-dimensional uniaxial XY model. In the \((R, T_c(R))\) plane, we have represented by a continuous line the locus of critical points separating the disordered (paramagnetic) phase from the ordered (ferromagnetic and modulated) phases. In the scale of the figure, the uncertainties of the points are smaller than the width of the line. The Lifshitz point (LP) is located at the intersection of the critical and the disorder line (represented by a dashed curve). A transition line, also expected to be of second order, separates the modulated from the ferromagnetic phase, and joins the Lifshitz point to the point \((R = -1/4, T = 0)\), where the ordering of the ground state changes. This line cannot be mapped out by HT methods and therefore is only schematically indicated by a sequence of open circles.
FIG. 2: A representation of the modified-ratio sequences \((K_{1c}(R))_n\) obtained from eq.(17). For a few values of \(R\) chosen in a vicinity of \(R_M\), the sequences have been extrapolated to large order by fitting them to the asymptotic form \(b_1(R) - b_2(R)/n^{1+\omega}\) with \(\omega = 0.52\). We have then plotted the modified-ratio sequences vs \(x = 1/n^{1+\omega}\), after normalizing them to their limiting values \(b_1(R)\). The elements of the normalized sequences are represented by open triangles and are connected by continuous lines to guide the eye. The corresponding best fits to the asymptotic form: 1. \(-a(R)/n^{1+\omega}\) with \(a(R) = b_2(R)/b_1(R)\) are represented by straight continuous lines.

TABLE I: Values of the critical exponents for the \((m, d, N) = (1, 3, 2)\) (uniaxial XY) Lifshitz point in three dimensions. The column with heading MF, taken from Ref.[50] reports the mean field exponents. In the column with heading \(O(\epsilon^2)\), we report the values obtained\(^\ddagger\) by evaluating at \(\epsilon = 3/2\) the \(\epsilon\)-expansions of the exponents truncated at the second order. Under the heading HT we report the results directly obtained in this paper. The heading MC refers to the results of the simulations in Refs.[46,47].

| Exponent | MF | \(O(\epsilon^2)\) | HT | MC |
|----------|----|----------------|----|----|
| \(\gamma_l\) | 1  | 1.495  | 1.535(25) | 1.5(1) |
| \(\nu_{\parallel}\) | \(\frac{1}{4}\) | 0.372 | 0.40(3) |
| \(\nu_{\perp}\) | \(\frac{1}{4}\) | 0.757 | 0.805(15) |
| \(\eta_{\parallel}\) | 0  | -0.020 | |
| \(\eta_{\perp}\) | 0  | 0.042 | |
| \(\alpha_l\) | 0  | -0.047 | |
| \(\beta_l\) | \(\frac{1}{2}\) | 0.276 | |
| \(\delta_l\) | 3  | 0.725 | 1.00(4) |
| \(\phi_l\) | \(\frac{1}{2}\) | 0.521 | 0.40(2) |
| \(\beta_q\) | \(\frac{1}{2}\) | 0.521 | 0.40(2) |
FIG. 3: The exponents $\gamma(R)$ and $\nu_\perp(R)$ (notice that for $R \gtrsim 0$ $\nu_\perp = \nu$) are computed along the $P-F$ branch of the critical line $K_{1c} = K_{1c}(R)$ in order to display their universality with respect to $R$. The horizontal continuous lines are bands of 0.5 % deviation from the central values, indicated by dashed lines, of recent high-precision estimates of the exponents $\gamma$ (in the case of the upper band), $\nu$ (central band, shifted upwards by 0.6) and of the ratio $\nu/\gamma$ (lower band shifted upwards by 0.7) for the XY universality class. We have indicated by open circles our estimates of the exponent $\gamma(R)$ obtained from DAs biased with the critical temperature, while the estimates obtained by the critical-point renormalization method, generally subject to a larger uncertainty, are denoted by open triangles. In the case of the exponent $\nu_\perp(R)$ we have denoted by open rhombs the estimates obtained from DAs biased with the critical temperature and by open squares the estimates obtained by the critical-point renormalization method. As already noticed, for graphical convenience, the values of this exponent are shifted upwards by 0.6. Finally a sequence of stars denotes the ratios $\nu_\perp(R)/\gamma(R)$ which, again for convenience, are shifted upwards by 0.7. A sequence of crosses schematically indicates a quantity proportional to the the absolute value $|a_\chi^+(R)|$ of the correction-to-scaling amplitude. For graphical convenience, this quantity is shifted upwards by 1.4. The vertical dashed line on the left-hand side indicates the value $R_{LP} = -0.2733(5)$ corresponding to the LP.
FIG. 4: A slightly modified and blown up representation of some of the data appearing in Fig. 3. We report the exponents $\gamma(R)$ (open circles), $\nu_(R)$ (open squares) and the ratio $\nu_\perp(R)/\gamma(R)$ (open triangles) computed by temperature-biased DAs along the $P-F$ branch of the critical line $K_{1c} = K_{1c}(R)$. The data are now normalized to the central values of the corresponding comparison estimates of the exponents for the XY universality class. The horizontal solid lines are bands of 0.5 % deviation from the comparison value (central dashed line). The vertical dashed line on the left-hand side indicates the value of $R_{LP}$. The upper curve, schematically denoted by crosses, plots a quantity proportional to the absolute value $|a^+_X(R)|$ of the correction-to-scaling amplitude. This quantity is shifted upwards by 1.01 for graphical convenience.

TABLE II: The critical values of $K_1$ for selected values of $R$. The uncertainties reported here correspond only to the spread of the DA estimates and therefore are likely to underestimate the real errors when $|R - R_M|$ is not small, particularly so for $R \lesssim 0$.

| $R$  | $K_{1c}(R)$ | $R$  | $K_{1c}(R)$ |
|------|-------------|------|-------------|
| 1.200| 0.15239(4)  | 0.500| 0.18429(1)  |
| 1.100| 0.15596(4)  | 0.400| 0.19075(1)  |
| 1.00 | 0.15980(4)  | 0.300| 0.19799(1)  |
| 0.900| 0.16391(3)  | 0.200| 0.20623(1)  |
| 0.800| 0.16836(3)  | 0.100| 0.21577(1)  |
| 0.700| 0.17319(2)  | 0.000| 0.22710(2)  |
| 0.600| 0.17847(2)  |-0.100| 0.24113(4)  |
FIG. 5: Same as Fig. 4, but here the exponents $\gamma(R)$ (open circles) and $\nu_\perp(R)$ (open squares) are computed along the $P-F$ branch of the critical line by DAs biased with $K_{1c}(R) + \delta K_{1c}(R)/2$ for $R > R_M + 0.03$ or biased with $K_{1c}(R) - \delta K_{1c}(R)/2$ for $R < R_M - 0.03$. Like in Fig. 4, the exponents are normalized to the mentioned comparison central values $\gamma = 1.3178$ and $\nu = 0.6717$, respectively. The horizontal solid lines are bands of 0.5% deviation from the central value indicated by a dashed line. The vertical dashed line indicates the value of $R_{LP}$. The sequence of crosses represents a quantity proportional to the absolute value $|a^{\chi}(R)|$ of the correction-to-scaling amplitude (shifted upwards by 1.01 for graphical convenience).
FIG. 6: Universality with respect to $R$ of the moment ratios $Q(p,q;r,s;R)$. We have reported results for $Q(1/2,1/2;0,1;R)$ represented by circles, for $Q(1/2,1/4;0,3/4;R)$ (triangles) and for $Q(1/2,1/2;1/4,3/4;R)$ (rhombus). The ratios are normalized to their values at $R_M$. The values of these ratios at $R_M$ are respectively: $Q(1/2,1/2;0,1;R_M) = 0.876(1)$, $Q(1/2,1/4;0,3/4;R_M) = 0.929(1)$ and $Q(1/2,1/2;1/4,3/4;R_m) = 0.9695(1)$. The sequence of crosses represents a quantity proportional to the absolute value $|a_\chi^+(R)|$ of the correction-to-scaling amplitude (and is shifted upwards by 1.01 for graphical convenience). The vertical dashed line indicates the value of $R_{LP}$. 


FIG. 7: The correlation function $C(0, 0; 0, 0, d)$ between the spin at the origin and a spin on the z-axis as a function of the distance $d$ between the spins, at fixed values of $R$ and $T$. We have chosen the value $(R = 0.11, T_c(R)/2 = 2.59)$ (open circles) on the right-hand of the disorder line and the value $(R = -1.0, T_c(R)/2 = 2.439)$ (open triangles) on the left-hand of it, to display the different behavior of the corresponding correlation function (pure exponential decay and oscillating exponential decay respectively). The lines connecting the symbols are drawn as a guide for the eye.
FIG. 8: The energy (upper curve), the $nn$-spin correlation function (middle curve) and the $nnn$-spin correlation function (lowest curve) computed near the boundary of the paramagnetic phase (at $T = 1.1T_c(R)$) and plotted vs $R$. The vertical dashed line indicates the value of $R_{LP}$. 
FIG. 9: The exponent $\gamma(R)$ computed along the $P-M$ branch of the critical line. The estimates obtained by the critical-point renormalization method are represented as open triangles, those obtained by DAs biased with the critical temperature as open circles. The horizontal continuous lines represent the values of the exponent $\gamma$ for the $O(2)$ (lowest line), $O(3)$ (intermediate line) and $O(4)$ (upper line) universality classes. The vertical dashed line indicates the value of $R_{LP}$. 
FIG. 10: The peak value of the modulation vector $\bar{q}_z$ at the critical temperature plotted vs. $R$ for $R \leq R_{LP}$. The continuous curve represents the mean-field prediction $\bar{q}_z^{MF} = \cos^{-1}(R_{LP}^{MF}/R)$ with $R_{LP}^{MF} = -1/4$. 