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The t-expansion study of critical phenomena in quantum systems

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Abstract. For quantum systems in the ground state, the t-expansion technique is used to construct a canonical sequence of classical theories. The consequent application of the coherent-anomaly method provides an estimation of the non-classical values of critical indices related to the singular behaviour of the ground-state energy. The accuracy of the results is tested on the Ising model with a transverse field, formulated on two- and three-dimensional lattices.

1. Introduction

Critical phenomena remain one of the most important topics in quantum and statistical mechanics. Subjects like universality breaking in some low-dimensional systems and the possibility of the restoration of universality below the upper critical dimension, the effect of randomness on the critical behaviour, etc, are still obscured in many relevant aspects. The greatest progress in studying non-integrable systems has been made by numerical methods, in particular the Monte Carlo simulations, the finite-size-scaling method and the extrapolation of low-temperature (weak-coupling) or high-temperature (strong-coupling) series into the critical region. Their common negative features are the laboriousness, the large amount of computer time needed even for a small system size, the application of specific algorithms in dependence on the particular family of models (e.g. the series expansions are done up to a sufficiently high perturbation order only for a few quantum Hamiltonians which symmetries allow for a simple graphical representation of series contributions), the uncertainty of qualitative predictions because of the entirely numerical character of the methods. It is therefore desirable to develop alternative analytic closed-form approaches based on physical considerations and self-consistency requirements, if need be in combination with series expansions within a variational format. However, such methods provide, at each approximation level, the classical critical description of systems with classical values of critical indices independent of dimension.

The problem of the restricted classical description is unravelled in the coherent anomaly method (CAM) [1] (for a recent review, see [2]). The main tool of the CAM is a successive sequence of classical-type theories which is canonical, i.e. gives critical points converging to the exact one. The non-classical corrections to the classical values of critical indices are deduced from a successive growth of prefactors to the corresponding (classical) singular parts of quantum or statistical quantities. The canonical series of approximations were practically generated within various cluster theories [3–5] (by increasing the cluster size,

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with a fixed number of effective fields) or alternative multi-effective-field schemes [6] (by varying the set of multi-body effective fields inside one fixed cluster).

This paper deals in the above spirit with the non-classical critical phenomena of quantum lattice models in the ground state. As the method of constructing a canonical sequence of approximations we use the non-perturbative t-expansion technique [7–10]. The last is close to the standard variational method, and improves the choice of a trial wavefunction by letting it evolve in time t; the t-expansion has been applied mostly to the calculation of molecule spectra and quite recently to the antiferromagnetic regime of the spin-$\frac{1}{2}$ Heisenberg model [11]. The essential practical advantage of the generated canonical series, which falls into the cluster-expansion category, is that one can obtain higher-level approximations relatively easily.

To accomplish our program, we proceed in three steps:

(i) The ambiguous part of the t-expansion technique is the extrapolation of the small-t series expansion to asymptotically large t; a summary of the known extrapolation procedures is given in [9]. We have observed that while the value of the ground-state energy depends negligibly on the type of extrapolation, the critical description is always inadequate—the generated series of approximations even lose the canonicality. That is why we propose a new extrapolation scheme, an improved version of the Stubbin's inverse method [9], which keeps all the required analytic properties of the t-expansion and gives reliable critical data (section 2).

(ii) We define precisely how the trial function controls the phases, and extract explicitly the leading term of the classical singular behaviour of the order parameter and of the susceptibility around the critical point (section 3).

(iii) As a test model we present the quantum Ising model in a transverse field (TIM), formulated on two-dimensional (2D) and three-dimensional (3D) lattices. The estimates of the critical point and of the non-classical values of critical indices β, γ, obtained by using the CAM, are consistent with the most reliable series results (section 4).

2. A sketch of the t-expansion method

The t-expansion technique [7] is based on the following theorem: for any trial ket $|\phi\rangle$ which has non-zero overlap with the exact ground-state $|0\rangle$ of a quantum system characterized by Hamiltonian $\hat{H}$, the state

$$|\phi_t\rangle = \frac{1}{\langle\phi|\mathrm{e}^{-t\hat{H}}|\phi\rangle^{1/2}}\mathrm{e}^{-t\hat{H}/2}|\phi\rangle \tag{2.1}$$

is a better approximation to $|0\rangle$ for any positive t and it tends to $|0\rangle$ in the limit $t \to \infty$. Consequently, the function

$$E(t) = \frac{\langle\phi|\hat{H}\mathrm{e}^{-t\hat{H}}|\phi\rangle}{\langle\phi|\mathrm{e}^{-t\hat{H}}|\phi\rangle} = \sum_{n=0}^{\infty}\frac{(-t)^n}{n!}I_{n+1} \tag{2.2}$$

converges to the ground-state energy E_0 at asymptotically large t. Here, the coefficients I_n, referred to as connected moments, are recursively defined by

$$\begin{aligned} I_1 &= \langle\phi|\hat{H}|\phi\rangle \\ I_n &= \langle\phi|\hat{H}^n|\phi\rangle - \sum_{p=0}^{n-2}\binom{n-1}{p}I_{p+1}\langle\phi|\hat{H}^{n-p-1}|\phi\rangle \qquad n \geqslant 2. \end{aligned} \tag{2.3}$$

They are size-extensive, i.e. for a large system of N units I_n scales like N. Since the derivative of $E(t)$ with respect to t is equal to the negative of the expectation value of

$(H - \langle\phi|H|\phi\rangle)^2$, $E(t)$ decreases *monotonously* from its initial (variational) value $I_1 > E_0$ to E_0 at $t \to \infty$, i.e. for any finite t, $E(t)$ is an upper bound for E_0.

In general, one can compute exactly only the first few coefficients $\{I_n\}$ of the small-t expansion (2.2). A non-trivial task is then to 'guess' the large-t behaviour of E: the set of free parameters in a suggested extrapolation formula is determined uniquely by comparing with (2.2) up to the given power of t. Various extrapolation schemes were examined, like the Padé and D-Padé approximants [7], connected-moments expansion (CMX) [8], extended-connected-moment expansion, Laplace and inversion methods [9]. The extensively used CMX method represents e.g. a finite-L truncation ($L = 0, 1, \ldots$) of an infinite series of exponentials,

$$E(t) = E_0 + \sum_{n=1}^{L} A_n \mathrm{e}^{-t/\alpha_n}. \tag{2.4}$$

The corresponding estimate of the ground-state energy density $\mathcal{E} = E_0/N$ is given by

$$\mathcal{E}_{2L+1} = \frac{1}{N}(I_1 - \boldsymbol{X}_L \boldsymbol{T}_L^{-1} \boldsymbol{X}_L^{\mathrm{T}}) \tag{2.5}$$

where $\boldsymbol{X}_L$ is the vector $(I_2, \ldots, I_{L+1})$ and $\boldsymbol{T}_L$ the matrix with elements $(T_L)_{ij} = I_{i+j+1}$ $(i, j = 1, \ldots, L)$; explicitly,

$$\mathcal{E}_1 = \frac{1}{N} I_1 \tag{2.6a}$$

$$\mathcal{E}_3 = \frac{1}{N}\left(I_1 - \frac{I_2^2}{I_3}\right) \tag{2.6b}$$

etc. The subscript of $\mathcal{E}$ denotes the approximation order = the number of the highest connected moment involved in the calculation of the ground-state energy. We have observed in our computations that while the value of approximative $\mathcal{E}$ depends only slightly on the type of extrapolation, the description of critical properties of the system in the ground state (based on the response of $\mathcal{E}$ under an infinitesimal change of the trial wavefunction $|\phi\rangle$—see the next section for an explanation) is very sensitive on the choice of extrapolation. From this point of view, all known methods give unstable and poorly convergent results. Here, we propose a new extrapolation scheme, a version of the inverse method [9], which keeps the relevant analytic properties of the plot $E(t)$ and gives quickly convergent and adequate critical data.

Let us first suppose that the monotonous decay of $E(t)$ from I_1 to E_0 is given by the only exponential in (2.4):

$$E(t) = E_0 + (I_1 - E_0)\mathrm{e}^{-t/\alpha}. \tag{2.7}$$

Then, the inverse function reads

$$t(E) = -\alpha \ln\left(\frac{E - E_0}{I_1 - E_0}\right) \tag{2.8}$$

and its derivative

$$\frac{\mathrm{d}t}{\mathrm{d}E} = -\frac{\alpha}{E - E_0} \tag{2.9}$$

exhibits a simple pole just at $E = E_0$. The r.h.s. of equation (2.9) is nothing but the leading term of the Laurent series expansion of the true $\mathrm{d}t/\mathrm{d}E$ around $E = E_0$, written as

$$\frac{\mathrm{d}t}{\mathrm{d}E} = -\frac{\alpha}{E - E_0} + \sum_{n=0}^{\infty} \frac{c_{n+1}}{n!}(E - E_0)^n \tag{2.10}$$

so that

$$t(E) = -\alpha \ln(E - E_0) + \sum_{n=0}^{\infty} \frac{c_n}{n!}(E - E_0)^n. \tag{2.11}$$

Let us now consider a finite truncation of (2.11):

$$t(E) = -\alpha \ln(E - E_0) + \sum_{n=0}^{L-3} \frac{c_n}{n!}(E - E_0)^n. \tag{2.11$'$}$$

The L unknown parameters $E_0, \alpha, \{c_n\}_{n=0}^{L-3}$ are determined by comparing the values of $t(E)$ and of its first $(L-1)$ derivatives with respect to E at point $E = I_1$, expressed in terms of the connected moments by inverting relation (2.2)

$$\begin{aligned} & t(E = I_1) = 0 \\ & d_E t(E = I_1) = -\frac{1}{I_2} \\ & d_{EE} t(E = I_1) = \frac{I_3}{I_2^3} \\ & d_E^{(3)} t(E = I_1) = \frac{I_2 I_4 - 3I_3^2}{I_2^5} \end{aligned} \tag{2.12}$$

etc, with those yielded by (2.11$'$). The resulting set of equations

$$\begin{aligned} & 0 = -\alpha \ln(I_1 - E_0) + \sum_{n=0}^{L-3} \frac{c_n}{n!}(I_1 - E_0)^n \\ & d_E t(I_1) = -\frac{\alpha}{I_1 - E_0} + \sum_{n=0}^{L-4} \frac{c_{n+1}}{n!}(I_1 - E_0)^n \\ & \vdots \\ & d_E^{(L-3)} t(I_1) = (-1)^{L-3} \frac{\alpha(L-4)!}{(I_1 - E_0)^{L-3}} + c_{L-3} \\ & d_E^{(L-2)} t(I_1) = (-1)^{L-2} \frac{\alpha(L-3)!}{(I_1 - E_0)^{L-2}} \\ & d_E^{(L-1)} t(I_1) = (-1)^{L-1} \frac{\alpha(L-2)!}{(I_1 - E_0)^{L-1}} \end{aligned} \tag{2.13}$$

implies the ground-state energy density of the form

$$\mathcal{E}_L = \frac{1}{N}\left[I_1 + (L-2)\frac{d_E^{(L-2)} t(I_1)}{d_E^{(L-1)} t(I_1)} \right]. \tag{2.14}$$

Since $d_E^{(n)} t(I_1)$ scales like N^{-n} (see equations (2.12)), $\mathcal{E}_L$ is size-intensive as was expected. In the lowest $L = 3$ order, we recover the CMX result (2.6b). However, while in higher truncation orders the CMX theory fits the decay of $E(t)$ by a linear combination of several exponentials, our method corresponds to a polynomial 'deformation' of one exponential. Since $\mathrm{d}t/\mathrm{d}E$ has just one simple pole by construction, the monotonous decay of $E(t)$ to E_0 at $t \to \infty$ is automatically ensured at every truncation level (in contrast to the CMX approach where some A's in (2.4) can be negative). The fundamental difference between the presented and the original [9] inverse methods is that here the inverse function $t(E)$ is uniquely built around $E = I_1$, and not around $E = 0$ which leads to an ambiguous choice of the polynomial branch.

3. General description of critical properties

The connected moments $\{I_n\}$, and consequently the value of $\mathcal{E}_L$ for finite L, depend on the choice of the trial function $|\phi\rangle$, besides an evident dependence on a complete list of Hamiltonian's parameters denoted by $\{J\}$. For lattice spin-$\frac{1}{2}$ systems we shall concentrate on, the set of trial functions will be parametrized by some free gauge parameter ϕ (the extension of the formalism to higher spins requiring the introduction of more gauge parameters is straightforward). The trivial lowest-order estimate (2.6a), $\mathcal{E}_1 = I_1(\{J\}, \phi)/N$, is the basic formula of the ordinary variational method, with $\mathcal{E}_1$ being a rigorous upper bound for the true $\mathcal{E}$. The 'best' value of ϕ is thus determined by the stationarity condition $\partial\mathcal{E}_1/\partial\phi = 0$; from all solutions to this condition the accepted (physical) one $\bar{\phi}$ provides the minimum of $\mathcal{E}_1$.

In higher L-orders of an extrapolation scheme, the corresponding estimates of the ground-state energy density $\mathcal{E}_L(\{J\}, \phi)$ are not rigorous upper bounds for the true $\mathcal{E}$. But one can still formulate a natural extension of the variational method using the following arguments. It is clear that if the limit $\lim_{L\to\infty} \mathcal{E}_L$ exists, then it does not depend on the gauge ϕ. On the other hand, the way in which the series approaches its limiting value certainly does. This is the main point: we have to choose ϕ such that it makes the series properly convergent. It turns out that for a fixed set of model's parameters $\{J\}$ there exists a region of moderate values of ϕ in which $\mathcal{E}_L$, as a function of ϕ, exhibits a plateau, while outside of this interval it oscillates with a growing amplitude—the sign of the loss of series convergence. In order to restore at least the 'local independence' on the gauge parameter, we impose the stationarity condition

$$\frac{\partial}{\partial\phi}\mathcal{E}_L(\{J\}, \phi) = 0 \tag{3.1}$$

taken as an implicit definition of ϕ as a function of Hamiltonian's parameters. From all roots to (3.1) localized in the above-mentioned interval of well-behaved ϕ, $S = \{\phi_i\}$, we choose the solution, $\bar{\phi}$, which provides the minimum for $\mathcal{E}_L$:

$$\mathcal{E}_L(\{J\}) = \mathcal{E}_L(\{J\}, \bar{\phi}_L) = \min_{\phi_i \in S} \mathcal{E}_L(\{J\}, \phi_i). \tag{3.2}$$

We shall call $\bar{\phi}_L(\{J\})$ the physical solution to the stationarity condition (3.1).

For a given L, the closed-form approximation, $\mathcal{E}_L$, represents a classical-type theory. The phase transitions and the critical behaviour are governed by the singularities of $\bar{\phi}_L$ which plays the role of an effective field. Like for instance, a first-order phase transition takes place when, by changing the model's parameters, the role of the physical stationarity solution is transferred from one root, ϕ_1, to the other, ϕ_2, such that $\phi_2 \neq \phi_1$: $\bar{\phi}$ exhibits a jump, $\phi_1 \to \phi_2$, at the transition point, and gives rise to the discontinuity of the first derivative of the ground-state energy. A second-order phase transition results from the coalescence of the above physical roots, ϕ_1 tends to ϕ_2 (the stationarity condition has a degenerate solution).

In order to derive explicitly the criticality condition, we specify the system symmetry (which is broken in the ordered phase) by introducing the unitary operator $\hat{T}$,

$$|\phi\rangle \to |\phi'\rangle = \hat{T}|\phi\rangle \tag{3.3}$$

which commutes with the Hamiltonian, $[\hat{T}, \hat{H}] = 0$. The unitary transformation (3.3) leaves the moments of the Hamiltonian invariant,

$$\langle\phi'|\hat{H}^n|\phi'\rangle = \langle\phi|\hat{H}^n|\phi\rangle. \tag{3.4}$$

Without any loss of generality, it is convenient to parametrize the set of trial functions in such a way that it holds that $\phi' = -\phi$. Consequently, $\mathcal{E}_L(\{J\},\phi) = \mathcal{E}_L(\{J\},-\phi)$ and the stationarity condition (3.1) is always satisfied at $\phi = 0$. Seeing that $|\phi = 0\rangle$ is the eigenstate of $\hat{T}$, $\bar{\phi}_L = 0$ is the physical gauge in the whole disorder region where $\mathcal{E}_L(\{J\},\phi)$ exhibits the minimum at $\phi = 0$. This minimum changes to the local maximum just at the critical point, determined by the criticality condition

$$\partial_{\phi\phi}\mathcal{E}_L(\{J^c\},\phi)|_{\phi=0} = 0 \tag{3.5}$$

with $\{J^c\}$ being the critical values of $\{J\}$. The stationarity root $\phi = 0$ is three-fold degenerate at the critical point, and the conjugate physical solutions $\bar{\phi}_L, -\bar{\phi}_L$ (providing identical minima of $\mathcal{E}_L$) split continuously from 0 inside the ordered phase region.

To calculate explicitly the classical singularities of ground-state quantities, we generalize the definition of $\mathcal{E}_L$ by introducing the order-parameter operator $\hat{s}$, satisfying $T\hat{s}|\phi\rangle = -\hat{s}|-\phi\rangle$ and coupled to a symmetry-breaking field h, into the Hamiltonian

$$\hat{H} \to \hat{H}(\{J\},h) \equiv \hat{H}(\{J\}) - h\hat{s}. \tag{3.6}$$

The corresponding $\mathcal{E}_L(\{J\},h;\phi)$ possesses the evident symmetry property

$$\mathcal{E}_L(\{J\},h;\phi) = \mathcal{E}_L(\{J\},-h;-\phi). \tag{3.7}$$

The spontaneous order parameter per site and the zero-field susceptibility are given by

$$s_L(\{J\}) = \lim_{h\to 0^+}\frac{\mathrm{d}}{\mathrm{d}h}[-\mathcal{E}_L(\{J\},h;\bar{\phi}_L)] \tag{3.8a}$$

$$\chi_L(\{J\}) = \lim_{h\to 0^+}\frac{\mathrm{d}^2}{\mathrm{d}h^2}[-\mathcal{E}_L(\{J\},h;\bar{\phi}_L)] \tag{3.8b}$$

respectively, where $\bar{\phi}_L = \bar{\phi}_L(\{J\},h)$ is the physical stationarity root on the extended parameter space. $\mathcal{E}_L(\{J\},h;\phi)$ is an analytic function of its arguments everywhere, including the critical region. With respect to the criticality condition (3.5) and the symmetry relation (3.7), its Taylor expansion around the critical point $(\{J^c\}, h = 0, \phi = 0)$ in powers of $\mathrm{d}J = J - J_L^c, h, \phi$, reads

$$\begin{aligned}\mathcal{E}_L(\{J\},h;\phi) = {}& \mathcal{E}_L(\{J^c\},0;0) + \sum_n(\partial_{J_n}\mathcal{E}_L)|_c\,\mathrm{d}J_n \\ & + \tfrac{1}{2!}\sum_{n,m}(\partial_{J_nJ_m}\mathcal{E}_L)|_c\,\mathrm{d}J_n\,\mathrm{d}J_m + (\partial_{h\phi}\mathcal{E}_L)|_c h\phi \\ & + \tfrac{1}{2!}\sum_n(\partial_{J_n\phi\phi}\mathcal{E}_L)|_c\,\mathrm{d}J_n\phi^2 + \sum_n(\partial_{J_nh\phi}\mathcal{E}_L)|_c\,\mathrm{d}J_n\,h\phi \\ & + \tfrac{1}{4!}(\partial_{\phi\phi\phi\phi}\mathcal{E}_L)|_c\phi^4 + \tfrac{1}{3!}(\partial_{h\phi\phi\phi}\mathcal{E}_L)|_c h\phi^3 + \ldots\end{aligned} \tag{3.9}$$

where the symbol $|_c$ means that the derivatives should be taken at the critical point. We have omitted in (3.9) all terms of orders higher than $(\mathrm{d}J)^2$ or h, regarding the leading classical singularities of ϕ, $\phi \sim (\mathrm{d}J)^{1/2}$ for $h = 0$ and $\phi \sim h^{1/3}$ for $\mathrm{d}J = 0$ (see the next text). For $h \to 0$, the application of the stationarity condition (3.1) to (3.9) results in

$$\sum_n(\partial_{J_n\phi\phi}\mathcal{E}_L)|_c\mathrm{d}J_n\phi + \tfrac{1}{3!}(\partial_{\phi\phi\phi\phi}\mathcal{E}_L)|_c\phi^3 + \ldots = 0. \tag{3.10}$$

Besides the trivial (disorder) solution $\phi = 0$, equation (3.10) implies two singular ones

$$\phi_L^{(1,2)} \simeq \pm\left[-\frac{6\sum_n(\partial_{J_n\phi\phi}\mathcal{E}_L)|_c\,\mathrm{d}J_n}{(\partial_{\phi\phi\phi\phi}\mathcal{E}_L)|_c}\right]^{1/2}. \tag{3.11}$$

They become physical in the symmetry-broken phase, characterized by the positivity of the expression in the square bracket. The prefactor sign is put to be identical to that of the vanishing field h in order to minimize $\mathcal{E}_L$. According to (3.8a), the leading singular part of the spontaneous order parameter takes the form

$$s_L \simeq -(\partial_{h\phi}\mathcal{E}_L)|_c \left[-\frac{6\sum_n (\partial_{J_n\phi\phi}\mathcal{E}_L)|_c \, \mathrm{d}J_n}{(\partial_{\phi\phi\phi\phi}\mathcal{E}_L)|_c} \right]^{1/2}. \tag{3.12}$$

As concerns the susceptibility (3.8b), it can be written as

$$\chi_L(\{J\}, h) = -\left(\partial_h + \frac{\partial\bar{\phi}_L}{\partial h}\partial_\phi\right)\left(\partial_h + \frac{\partial\bar{\phi}_L}{\partial h}\partial_\phi\right)\mathcal{E}_L(\{J\}, h, \phi)\Big|_{\phi=\bar{\phi}_L}. \tag{3.13}$$

The derivative of $\bar{\phi}_L$ with respect to h is deducible from its implicit definition $\partial_\phi\mathcal{E}_L|_{\phi=\bar{\phi}_L} = 0$,

$$\frac{\partial\bar{\phi}_L}{\partial h} = -\frac{\partial_{h\phi}\mathcal{E}_L}{\partial_{\phi\phi}\mathcal{E}_L}\Big|_{\phi=\bar{\phi}_L}. \tag{3.14}$$

Consequently, the singular part of χ_L reads

$$\chi_L \simeq \frac{(\partial_{h\phi}\mathcal{E}_L)^2}{\partial_{\phi\phi}\mathcal{E}_L}\Big|_{\phi=\bar{\phi}_L}. \tag{3.15}$$

For $h = 0$ and in the disorder region ($\bar{\phi}_L = 0$) close to the critical point,

$$(\partial_{h\phi}\mathcal{E}_L)|_{\phi=\bar{\phi}_L} = (\partial_{h\phi}\mathcal{E}_L)|_c + \ldots \tag{3.16a}$$

$$(\partial_{\phi\phi}\mathcal{E}_L)|_{\phi=\bar{\phi}_L} = \sum_n (\partial_{J_n\phi\phi}\mathcal{E}_L)|_c \, \mathrm{d}J_n + \ldots \tag{3.16b}$$

so that

$$\chi_L^{\text{disorder}} \simeq \frac{(\partial_{h\phi}\mathcal{E}_L)^2|_c}{\sum_n (\partial_{J_n\phi\phi}\mathcal{E}_L)|_c \, \mathrm{d}J_n}. \tag{3.17}$$

In the symmetry-broken phase,

$$(\partial_{\phi\phi}\mathcal{E}_L)|_{\phi=\bar{\phi}_L} = \sum_n (\partial_{J_n\phi\phi}\mathcal{E}_L)|_c \, \mathrm{d}J_n + \tfrac{1}{2!}(\partial_{\phi\phi\phi\phi}\mathcal{E}_L)|_c\bar{\phi}_L^2 + \ldots. \tag{3.18}$$

Setting $\bar{\phi}_L = \phi_L^{(1,2)}$ (3.11), we finally find

$$\chi_L^{\text{order}} \simeq -\frac{1}{2}\frac{(\partial_{h\phi}\mathcal{E}_L)^2|_c}{\sum_n (\partial_{J_n\phi\phi}\mathcal{E}_L)|_c \, \mathrm{d}J_n} \tag{3.19}$$

i.e. when approaching the critical point from disordered and ordered phases, the respective divergent parts of χ_L differ from one another only by an L-independent constant (note that the minus sign in (3.19) ensures the positivity of χ_L—the deviations $\mathrm{d}J_n$ have opposite signs in the disordered and ordered regions). This fact and the value of the proportionality constant are consistent with the prediction of the renormalization group [12]. We add that the above extraction of the leading classical singularities is formally similar to the one presented in [13] for statistical systems (we refer the reader to this work for the physical interpretation of the gauge parameter as an effective field).

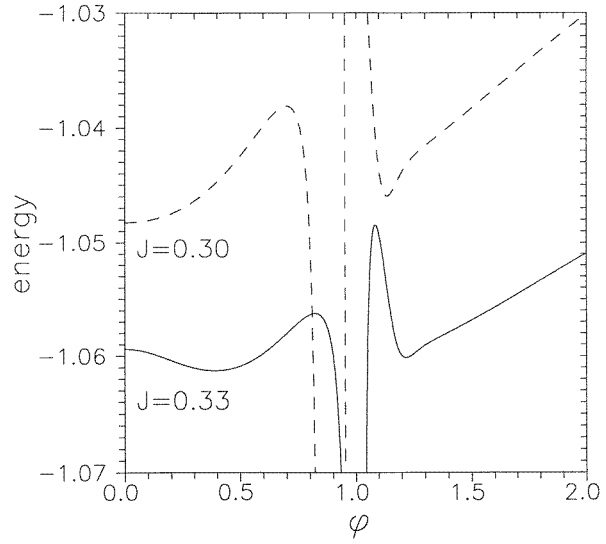

Figure 1. The plot of the ground-state energy versus the gauge parameter ϕ for the transverse Ising model on the square lattice; for details see the text.

4. Numerical results

We have performed the computations for the quantum TIM, defined by the Hamiltonian

$$\hat{H}(J) = -J \sum_{(n,m)} \sigma_n^z \sigma_m^z - \sum_n \sigma_n^x \tag{4.1}$$

and formulated on the 2D square, triangular and 3D simple cubic lattices; (n, m) denotes the nearest-neighbour couples of lattice points. Suzuki [14] proved the equivalence of the ground-state singularities of the TIM (4.1) formulated on a D-dimensional lattice to the singularities of the free energy of the classical spin-$\frac{1}{2}$ Ising model in $(D + 1)$ dimensions. The order parameter $\hat{s}$ is equal to $\sum_n \sigma_n^z$, the symmetry-broken phase corresponds to the ferromagnet and the symmetry operator $\hat{T}$ transforms each site-vector $a_n|\sigma_n^z = 1\rangle + b_n|\sigma_n^z = -1\rangle$ to $a_n|\sigma_n^z = -1\rangle + b_n|\sigma_n^z = 1\rangle$. The trial function is proposed simply as a direct product of one-site vectors

$$|\phi\rangle = \otimes_n \frac{1}{\sqrt{1+\mathrm{e}^{2\phi}}} \begin{pmatrix} 1 \\ \mathrm{e}^{\phi} \end{pmatrix} = \otimes_n \frac{1}{\sqrt{1+\mathrm{e}^{2\phi}}} (|\sigma_n^z = 1\rangle + \mathrm{e}^{\phi}|\sigma_n^z = -1\rangle). \tag{4.2}$$

The parametrization ensures $\hat{T}|\phi\rangle = |-\phi\rangle$.

Within the improved inverse method (formula (2.14)), we have expressed the functional dependence of the ground-state energy density $\mathcal{E}_L(J, \phi)$ up to the $L = 8$ (square lattice) and $L = 7$ (triangular, simple cubic lattices) approximation orders. For the case of the square lattice and $L = 7$, the plot of $\mathcal{E}_7$ as a function of the gauge parameter ϕ is drawn in figure 1 (we recall that $\mathcal{E}_L(\phi) = \mathcal{E}_L(-\phi)$): the broken curve corresponds to the disorder regime with the local minimum at $\phi = 0$, the full curve corresponds to the symmetry-broken phase with the local maximum at $\phi = 0$ and the local minimum at $\phi \neq 0$. The figure also documents the plateau structure of $\mathcal{E}$ close to $\phi = 0$; for ϕ greater than one the function exhibits singularities and oscillates uncontrollably.

The critical values of the coupling $\{J_L^c\}$, obtained with the aid of the criticality condition (3.5), are summarized in table 1. It is seen that by increasing the approximation order L the

Table 1. The critical values of the coupling J_L^c and the prefactors $\bar{s}_L, \bar{\chi}_L$ to the classical singularities (equations (4.3a) and (4.4a)) obtained at the approximation order L for the transverse Ising model defined on various lattices.

L	J_L^c	$\bar{s}_L$	$\bar{\chi}_L$
2D square lattice			
3	0.301 203 117	3.123 510 065	0.368 996 739
4	0.305 572 205	3.284 269 318	0.393 738 999
5	0.308 704 467	3.366 451 062	0.413 824 307
6	0.310 870 522	3.438 583 050	0.430 055 617
7	0.312 497 360	3.499 848 315	0.443 807 786
8	0.313 788 767	3.554 125 659	0.455 902 538
2D triangular lattice			
3	0.198 215 145	4.115 881 328	0.257 849 690
4	0.198 746 068	4.154 095 606	0.263 349 076
5	0.200 045 884	4.237 156 162	0.274 295 288
6	0.200 965 334	4.312 717 281	0.283 075 332
7	0.201 668 869	4.379 999 768	0.290 557 008
3D simple cubic lattice			
3	0.187 204 7784	3.680 359 9162	0.211 564 524
4	0.188 477 8323	3.755 274 4284	0.217 893 088
5	0.189 212 3943	3.788 458 6549	0.221 860 256
6	0.189 731 8966	3.819 677 8071	0.225 068 181
7	0.190 110 4969	3.845 186 9490	0.227 621 329

couplings $\{J_L^c\}$ tend systematically to their asymptotic value, which indicates the canonicality of the approximation series. For comparison, the CMX method (formula (2.5)) applied to the square lattice gives the results $J_1^c = 0.25$, $J_3^c = 0.301$, $J_5^c = 0.231$, etc—an evident loss of the canonicality property in the CMX format. To find the asymptotic value of the coupling constant $\lim_{L\to\infty} J_L^c = J^c$, we have fitted data by the third-order polynomial $J_L^c = J^c + a_1/L + a_2/L^2 + a_3/L^3$ (hereinafter, the lowest-order $L = 3$ points, lying too far from the true critical region, are excluded from the standard least-square fits). The values of J^c obtained for the considered lattices are presented in table 2, together with the estimates of various methods. The errors are guessed from other $1/L$ fittings of $\{J_L^c\}$-data, namely the first- and second-order polynomial fits, the power fit.

The formulae describing the classical singularities of the order parameter (3.12) and of the susceptibility (say in the disorder regime, equation (3.17)) now take the form

$$s_L \simeq \bar{s}_L (J - J_L^c)^{1/2} \tag{4.3a}$$

$$\bar{s}_L = -(\partial_{h\phi}\mathcal{E}_L)|_c \left[-\frac{6(\partial_{J\phi\phi}\mathcal{E}_L)}{(\partial_{\phi\phi\phi\phi}\mathcal{E}_L)}\bigg|_c \right]^{1/2} \tag{4.3b}$$

$(J > J_L^c)$, and

$$\chi_L^{\text{disorder}} \simeq \bar{\chi}_L \frac{1}{(J_L^c - J)} \tag{4.4a}$$

$$\bar{\chi}_L = -\frac{(\partial_{h\phi}\mathcal{E}_L)^2}{(\partial_{J\phi\phi}\mathcal{E}_L)}\bigg|_c \tag{4.4b}$$

$(J < J_L^c)$, respectively. Here, $\mathcal{E}_L$ is defined on the extended parameter space of the Hamiltonian $\hat{H}(J,h) \equiv \hat{H}(J) - h\sum_n \sigma_n^z$. The numerical values of the prefactors to the

Table 2. A comparison of the present results for the critical coupling with indices β, γ of the transverse Ising model with: WC = weak-coupling series, SC = strong-coupling series, FS = finite-size scaling; (b) = biased, (ub) = unbiased.

	J^c	β	γ
2D square lattice			
WC [15]	0.329(1)	—	1.25(2)
SC [16] (ub)	0.328 50(4)	—	1.245(3)
(b)	0.328 50(4)	—	1.244(3)
FS [17]	0.328(1)	—	1.24(2)
CAM [4]	0.327(4)	—	1.25(8)
Present work	0.326(3)	0.35(2)	1.27(4)
2D triangular lattice			
WC [15]	0.2098(2)	—	1.250(12)
SC [16] (ub)	0.209 72(2)	—	1.242(2)
(b)	0.20972(2)	—	1.241(3)
FS [17]	0.2098(2)	—	1.236(8)
Present work	0.207(3)	0.37(3)	1.24(3)
3D simple cubic lattice			
WC [18] (ub)	0.19406(6)	0.43(2)	1.17(6)
(b)	0.19406(6)	0.425(7)	1.11(5)
SC [18] (ub)	0.1940(4)	—	1.08(2)
(b)	0.1940(4)	—	1.086(8)
Present work	0.192(1)	0.45(1)	1.09(2)

classical singularities $\bar{s}_L, \bar{\chi}_L$ are presented in table 1. According to the CAM [1, 2], they are presumed to exhibit the anomalous behaviour

$$\bar{s}_L \sim (J^c - J_L^c)^{-\Delta\beta} \tag{4.5a}$$

$$\bar{\chi}_L \sim (J^c - J_L^c)^{-\Delta\gamma} \tag{4.5b}$$

as $J_L^c \to J^c$. The exponents $-\Delta\beta$ and $\Delta\gamma$ represent the respective corrections to the classical critical indices $\frac{1}{2}$ and 1:

$$\beta = \tfrac{1}{2} - \Delta\beta \tag{4.6a}$$

$$\gamma = 1 + \Delta\gamma. \tag{4.6b}$$

Figures 2 and 3 show in the logarithmic scale that our data closely follow very well the linear fitting predicted by the coherent-anomaly formulae (4.5a) and (4.5b). The results for the non-classical values of exponents β and γ are tabulated in table 2; the errors are yielded by the previously discussed uncertainty in the determination of J^c (the errors coming from the numerical differentiation and from the standard deviation of the data fitting turn out to be one order lower). We also present the estimates of β, γ, obtained by other methods for comparison. The best results are provided in general by the extrapolation of series [15, 16, 18]. The last are restricted to the susceptibility expansion for which a simple perturbation algorithm has been established. We see that our estimates lie near the best ones, their deviations being similar to those of the CAM results [4] when available (the critical point and the critical exponent are determined simultaneously there; when the critical point is determined independently the exponents are estimated with higher accuracy [19]).

Dimension three is the upper critical dimension for the considered quantum TIM, beyond which the critical behaviour is that of mean-field theory and there holds $\Delta\beta = \Delta\gamma = 0$.

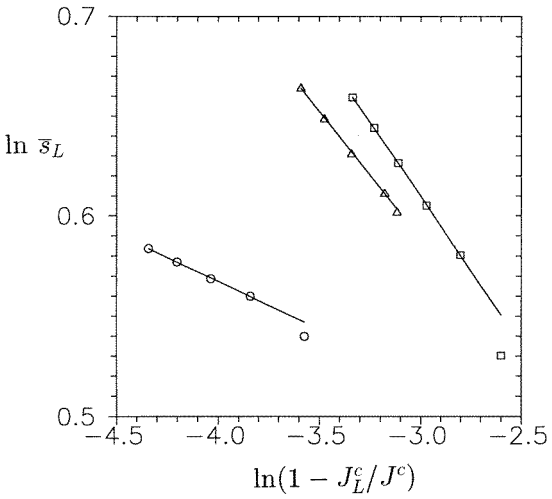

Figure 2. Magnetization prefactors $\bar{s}_L$ versus $(J_L^c - J^c)/J^c$ in the logarithmic scale for the square (□), triangular (△) and simple cubic (○) lattices (data for $\bar{s}_L$ have been uniformly scaled for every lattice structure in order to locate them in the same graph). Full lines correspond to the linear fits (the lowest $L = 3$ data are excluded from fittings), their slopes determine the correction to the classical index $\beta = \frac{1}{2}$.

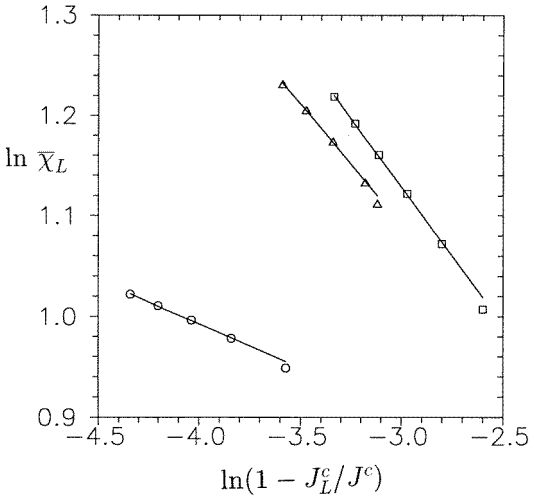

Figure 3. The same as figure 2 for the susceptibility data.

According to field-theoretical studies of the ϕ^4-model in four dimensions [12], the mean-field critical behaviour is modified by confluent logarithmic corrections. The $(3+1)$-dimensional TIM is expected to exhibit similar critical properties. Like for instance, the singular part of the order parameter is predicted in the form

$$s \sim (J - J^c)^{1/2}[-\ln(J - J^c)]^{1/3} \qquad \text{for } J \to J^c + . \tag{4.7}$$

We have put $\Delta\beta = 0$ and fitted the growth of the prefactors $\bar{s}_L$ according to the expected coherent-anomaly $\bar{s}_L \sim [-\ln(J^c - J_L^c)]^{\omega}$. The result $\omega = 0.27$ agrees with the predicted value at a reasonable level of accuracy.

5. Concluding remarks

In the present paper, we have put the t-expansion technique into an efficient mean for investigating, in combination with the idea of coherent anomaly, the non-classical critical properties of quantum systems in the ground state. The results for the TIM indicate a high reliability of the method which has some relevant advantages:

(1) in contrast to the conventional cluster approaches where the cluster size is equal to L^D at the approximation order L, the complexity of the connected-moment graphs grows very slowly with increasing spatial dimension D (connected graphs having the origin in dimensions $< D$, with adjusted topological factors, are dominant);

(2) it is possible to explicitly extract the singular parts of the ground-state quantities.

These are the main reasons why we were able to take into account larger clusters in higher dimensions without extensive computational efforts. We believe that the suitability of the method in higher dimensions permits one to attack some fundamental problems, for example, the phase structure of 2D strongly-correlated quantum systems, to answer whether the universality is restored in two dimensions for the XYZ Heisenberg model and so on. These are our tasks for the future.

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References

[1] Suzuki M 1986 *J. Phys. Soc. Japan* **55** 4205
[2] Suzuki M, Hu X, Hatano N, Katori M, Minami K, Lipowski A and Nonomura Y 1995 *Coherent Anomaly Method* (Singapore: World Scientific)
[3] Nonomura Y and Suzuki M 1992 *J. Phys. A: Math. Gen.* **25** 85
[4] Nonomura Y and Suzuki M 1992 *J. Phys. A: Math. Gen.* **25** 5463
[5] Nonomura Y and Suzuki M 1994 *J. Phys. A: Math. Gen.* **27** 1127
[6] Minami K, Nonomura Y, Katori M and Suzuki M 1991 *Physica* **174A** 479
[7] Horn D and Weinstein M 1984 *Phys. Rev.* D **30** 1256
[8] Cioslowski J 1987 *Chem. Phys. Lett.* **136** 515
[9] Stubbins C 1988 *Phys. Rev.* D **38** 1942
[10] Markoš P and Olejník Š 1990 *Phys. Rev.* D **42** 2943
[11] Lee K C and Lo C F 1994 *J. Phys.: Condens. Matter* **6** 7075
[12] Brezin E, Le Guillou J C and Zinn-Justin J 1976 *Phase Transition and Critical Phenomena* vol 6, ed C Domb and M S Green (New York: Academic)
[13] Kolesík M and Šamaj L 1993 *J. Stat. Phys.* **72** 1203
[14] Suzuki M 1976 *Prog. Theor. Phys.* **56** 1454
[15] Marland L G 1981 *J. Phys. A: Math. Gen.* **14** 2047
[16] He H X, Hamer C J and Oitmaa J 1990 *J. Phys. A: Math. Gen.* **23** 1775
[17] Henkel M 1987 *J. Phys. A: Math. Gen.* **20** 3969
[18] Weihong Z, Oitmaa J and Hamer C J 1994 *J. Phys. A: Math. Gen.* **27** 5425
[19] Minami K and Suzuki M 1993 *Physica* **195A** 457