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Finite-size scaling in the φ^4 theory above the upper critical dimension*

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Abstract. We derive exact results for several thermodynamic quantities of the $O(n)$ symmetric φ^4 field theory in the limit $n \to \infty$ in a finite d-dimensional hypercubic geometry with periodic boundary conditions. Corresponding results are derived for an $O(n)$ symmetric φ^4 model on a finite d-dimensional lattice with a finite-range interaction. The leading finite-size effects near T_c of the field-theoretic model are compared with those of the lattice model. For $2 < d < 4$, the finite-size scaling functions are verified to be universal. For $d > 4$, significant lattice effects are found. Finite-size scaling in its usual simple form does not hold for $d > 4$ but remains valid in a generalized form with two reference lengths. The finite-size scaling functions of the φ^4 field theory turn out to be nonuniversal whereas those of the φ^4 lattice model are independent of the nonuniversal model parameters. In particular, the field-theoretic model exhibits finite-size effects whose leading exponents differ from those of the lattice model. The widely accepted lowest-mode approach is shown to fail for both the field-theoretic and the lattice model above four dimensions.

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1 Introduction

Exactly solvable models play an important role in the statistical theory of phase transitions. Most interesting are models that exhibit phase transitions of a non-mean-field type. The spherical model [1–3] as well as $O(n)$ symmetric models in the limit $n \to \infty$ [4] are of particular interest as they can be solved exactly for general dimensions d and for a fully finite geometry [5–7]. This provides the opportunity for examining fundamental properties of general interest such as universality and finite-size scaling [3,8–12] for $d \leq d_u$ and $d > d_u$ where d_u is the upper critical dimension. A particular advantage is that these properties can be studied both in a field-theoretic and a lattice version of the φ^4 theory [13].

In a recent paper [13] we have presented the exact result for the order-parameter correlation function of the $O(n)$ symmetric φ^4 field theory for a finite d-dimensional cube with periodic boundary conditions in the limit $n \to \infty$. Here we present the derivation of this result and calculate other thermodynamic quantities in this limit. For comparison, corresponding results will be derived for an $O(n)$ symmetric φ^4 model on a finite d-dimensional lattice.

Our exact treatment of the field-theoretic φ^4 model in the large-n limit is performed at finite cutoff. Since no perturbative approximations are involved (whose applicability usually deteriorates near criticality) there is no need for invoking the renormalization group (whose task would be to map the perturbation results from the critical to the non-critical region where perturbation theory is applicable). Thus our treatment remains conceptually simple and avoids unnecessary complications of renormalized field theory.

Although the lattice models studied previously [5,6] contain essentially the same features as the φ^4 lattice model studied in the present paper we consider the latter model as most appropriate for the purpose of a direct comparison with the standard field-theoretic version of the φ^4 model. In particular, unlike the previous models [5,6], the φ^4 lattice model enables us to keep track of the different roles played by the four-point coupling $\hat{u}_0$ with regard to three aspects for $d > 4$: (i) the "dangerous irrelevant" character of $\hat{u}_0$ for $T \leq T_c$ [14–16], (ii) non-universal cut-off effects that are tied to $\hat{u}_0$ and that are important for $d > 4$, (iii) leading finite-size effects for $T > T_c$ proportional to $\hat{u}_0$ arising from the *inhomogeneous* order-parameter fluctuations. The aspects (ii) and (iii) have not been discussed previously in the context of finite-size theory. The last aspect (iii) will be important in comparing our solution with that of reference [6].

* Dedicated to J. Zittartz on the occasion of his 60th birthday

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The discussion of our results will be focused on the differences between the leading finite-size effects for the field-theoretic and the lattice model. For $2 < d < 4$, the finite-size scaling functions of the susceptibility, the order parameter and the specific heat are verified to be universal, *i.e.*, to be identical for the field-theoretic and the lattice model and to be independent of the form of the (finite-range) lattice interaction, apart from metric factors. For $d > 4$ significant lattice effects are found. Finite-size scaling in its usual simple form does not hold for $d > 4$, as found previously [5], but remains valid in a generalized form with two reference lengths. Here we find the unexpected result that the corresponding finite-size scaling functions have a different structure for the field-theoretic and the lattice model. In particular we confirm our recent result [13] that the exponents of the leading finite-size effects on thermodynamic quantities of the field-theoretic model differ from those of the lattice model. The finite-size scaling functions for the field-theoretic model are found to be nonuniversal for $d > 4$ whereas those of the φ^4 lattice model are independent of the nonuniversal model parameters. Our scaling form for the susceptibility of the φ^4 lattice model for $n \to \infty$ disagrees with a previous non-scaling result for a modified version of the mean spherical model [6,7] for $d > 4$.

Our results show that the lowest-mode approach [17] fails in describing the leading finite-size effects above four dimensions for the field-theoretic model [13]; for the lattice model, it fails for $T > T_c$. Thus the widely accepted arguments with regard to the irrelevance of inhomogeneous fluctuations for $d > 4$ [17] are not generally valid. This is of relevance to the interpretation of as yet unexplained Monte-Carlo data of the five-dimensional Ising-model [18].

2 Finite-size effects in the φ^4 field theory for $n \to \infty$

We start from the standard Landau-Ginzburg-Wilson Hamiltonian of the $O(n)$ symmetric φ^4 field theory

$$H = \int_V d^d x [\frac{1}{2} r_0 \varphi^2 + \frac{1}{2}\sum_{a=1}^{n} (\nabla \varphi_\alpha)^2 + u_0 (\varphi^2)^2] \quad (1)$$

for an n-component field $\varphi(\mathbf{x}) = (\varphi_1, \varphi_2, ..., \varphi_n)$ in a finite volume V where φ^2 stands for $\sum_{\alpha=1}^{n} \varphi_\alpha^2$. For simplicity we consider a d-dimensional cube, $V = L^d$, with periodic boundary conditions,

$$\varphi(\mathbf{x}) = L^{-d} \sum_{\mathbf{k}} \varphi_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (2)$$

The summation runs over discrete $\mathbf{k}$ vectors with components $k_j = 2\pi m_j/L, m_j = 0, \pm 1, \pm 2, ..., j = 1, 2, ... d$, in the range $-\Lambda \le k_j < \Lambda$ with a finite cutoff Λ. In terms of the Fourier components

$$\varphi_{\mathbf{k}} = \int_V d^d x e^{-i\mathbf{k}\cdot\mathbf{x}} \varphi(\mathbf{x}) \quad (3)$$

the Hamiltonian reads

$$H = L^{-d} \sum_{\mathbf{k}} \frac{1}{2}(r_0 + \mathbf{k}^2) \varphi_{\mathbf{k}} \varphi_{-\mathbf{k}} + u_0 L^{-3d} \sum_{\mathbf{k}\mathbf{k}'\mathbf{k}''} (\varphi_{\mathbf{k}} \varphi_{\mathbf{k}'})(\varphi_{\mathbf{k}''} \varphi_{-\mathbf{k}-\mathbf{k}'-\mathbf{k}''}). \quad (4)$$

We are interested in the large-n limit of the Gibbs free energy per unit volume and per component

$$f = -\frac{1}{nL^d} \ln Z \quad (5)$$

and of the correlation function

$$\chi = \frac{1}{n} \int_V d^d x \langle \varphi(\mathbf{x}) \varphi(0) \rangle \quad (6)$$

where

$$\langle \varphi(\mathbf{x}) \varphi(0) \rangle = \frac{1}{Z} \int \mathcal{D}\varphi \; \varphi(\mathbf{x}) \varphi(0) \exp(-H), \quad (7)$$

with the partition function

$$Z = \int \mathcal{D}\varphi \; \exp(-H). \quad (8)$$

As usual, the symbol $\int \mathcal{D}\varphi$ is an abbreviation for the multiple integral over the real and imaginary parts of (the finite number of) the Fourier components $\varphi_{\mathbf{k}}$. For $T \ge T_c$, χ can be interpreted as the susceptibility (per component) of the finite system.

It is well known that for the case of an infinite ($V \to \infty$) system [19,20] a saddle point approach can be employed in the limit $n \to \infty$. Here we apply this approach to the finite system. We introduce an auxiliary field $s(\mathbf{x})$ (that also satisfies periodic boundary conditions) and represent the $u_0(\varphi^2)^2$ term of H by a Gaussian integral over $s(\mathbf{x})$ according to the Hubbard-Stratonovitch transformation

$$\exp\left[-\int_V d^d x u_0 (\varphi^2)^2 \right] = \widetilde{A} \int \mathcal{D}s \exp\left[-\int_V d^d x \left(\frac{n}{2} s^2 - i\sqrt{2u_0 n}\, s \varphi^2 \right) \right]. \quad (9)$$

The constant $\widetilde{A}$ is finite and independent of $\varphi(\mathbf{x})$. Then the partition function becomes

$$Z = \widetilde{A} \int \mathcal{D}s \; \exp\left[-\frac{n}{2} \int_V d^d x s^2 \right] \; \widetilde{Z}(s) \quad (10)$$

where

$$\widetilde{Z}(s) = \int \mathcal{D}\varphi \, \exp\left[- \int_V d^d x \sum_{\alpha=1}^{n} \left(\frac{1}{2} r_0 \varphi_\alpha^2 - i \, \sqrt{2u_0 n} \, s(\mathbf{x}) \varphi_\alpha(\mathbf{x})^2 + \frac{1}{2} (\bigtriangledown \varphi_\alpha)^2 \right) \right] \quad (11)$$

consists of decoupled integrations over the n components φ_α of φ. Since each component contributes in the same way we have

$$\widetilde{Z}(s) = \left[\widetilde{Z}_1(s) \right]^n = \exp\left[-nL^d \widetilde{f}(s) \right] \quad (12)$$

with

$$\widetilde{f}(s) = -\frac{1}{L^d} \ln \int \mathcal{D}\widetilde{\varphi} \exp\left[- \int_V d^d x \left(\frac{r_0}{2} \widetilde{\varphi}^2 - i \sqrt{2u_0 n} \, s(\mathbf{x}) \widetilde{\varphi}(\mathbf{x})^2 + \frac{1}{2} (\bigtriangledown \widetilde{\varphi})^2 \right) \right] \quad (13)$$

where now $\widetilde{\varphi}(\mathbf{x})$ is a one-component field. The Gaussian integration over $\widetilde{\varphi}$ can be performed in the usual way [19-21]. The result depends on the field $s(\mathbf{x})$.

As suggested by the calculation in the bulk case [19,20] the integration over $s(\mathbf{x})$ in (10) is reduced, in the limit $n \to \infty$ at fixed $u_0 n$, to a substitution of a uniform ($\mathbf{x}$-independent) saddle point value $s(\mathbf{x}) = \bar{s}$. This value is determined by

$$\bar{s} + \frac{\partial}{\partial \bar{s}} \widetilde{f}(\bar{s}) = 0 \quad (14)$$

where

$$\widetilde{f}(\bar{s}) = \widetilde{f}_0 + \frac{1}{2L^d} \sum_{\mathbf{k}} \ln(r_0 - 2i\sqrt{2u_0 n} \, \bar{s} + \mathbf{k}^2), \quad (15)$$

thus

$$\bar{s} - i \frac{\sqrt{2u_0 n}}{L^d} \sum_{\mathbf{k}} \frac{1}{r_0 - 2i\sqrt{2u_0 n} \, \bar{s} + \mathbf{k}^2} = 0. \quad (16)$$

Similarly the correlation function (6) is determined in this limit by the exponential weight in (13) with $s(\mathbf{x}) = \bar{s}$, thus

$$\chi^{-1} = r_0 - 2i\sqrt{2u_0 n} \, \bar{s}. \quad (17)$$

This result is easily generalized to finite $\mathbf{k}$,

$$\chi(\mathbf{k}) = \frac{1}{n} \int d^d x e^{-i\mathbf{k}\cdot\mathbf{x}} \langle \varphi(\mathbf{x}) \, \varphi(0) \rangle. \quad (18)$$

In the large-n limit one obtains

$$\chi(\mathbf{k})^{-1} = \chi^{-1} + \mathbf{k}^2. \quad (19)$$

Substituting (17) into (15, 16) we finally obtain the Gibbs free energy $f = \bar{f}_0 + \frac{1}{2}\bar{s}^2 + \widetilde{f}(\bar{s})$ of the finite system as

$$f = f_0 - \frac{(r_0 - \chi^{-1})^2}{16 u_0 n} + \frac{1}{2} L^{-d} \sum_{\mathbf{k}} \ln(\chi^{-1} + \mathbf{k}^2) \quad (20)$$

where χ^{-1} is determined implicitly by [13]

$$\chi^{-1} = r_0 + 4u_0 n \, L^{-d} \sum_{\mathbf{k}} (\chi^{-1} + \mathbf{k}^2)^{-1} \quad (21)$$

and where $f_0 = \bar{f}_0 + \widetilde{f}_0$ is an unimportant constant.

For $T \geq T_c$, the bulk susceptibility follows from the bulk limit of (21) as

$$\chi_b^{-1} = r_0 + 4u_0 n \int_{\mathbf{k}} (\chi_b^{-1} + \mathbf{k}^2)^{-1} \quad (22)$$

where $\int_{\mathbf{k}}$ stands for $(2\pi)^{-d} \int d^d k$ with a finite cutoff $|k_j| \leq \Lambda$. The same equation determines the square of the bulk correlation length ξ above T_c in the large-n limit [19,21],

$$\xi^2 = \chi_b \left[\partial \chi_b(\mathbf{k})^{-1} / \partial \mathbf{k}^2 \right]_{\mathbf{k}=\mathbf{0}} = \chi_b. \quad (23)$$

This implies the relation between the bulk critical exponents $\gamma = 2\nu$ for general $d > 2$. At T_c ($\chi_b^{-1} = 0$) the bulk critical value of r_0 is obtained from (22) as

$$r_{0c} = -4u_0 n \int_{\mathbf{k}} \mathbf{k}^{-2} \quad (24)$$

which is finite for $d > 2$.

We also consider the quantity

$$M^2 = \frac{1}{nL^{2d}} \left\langle \left[\int_V d^d x \, \varphi(\mathbf{x}) \right]^2 \right\rangle \quad (25)$$

which for $L \to \infty$ becomes the square of the bulk order parameter [22] divided by n. From (6) we have for finite n and finite L

$$M^2 = L^{-d} \chi. \quad (26)$$

For the analysis of finite-size effects it will be important to separate the $\mathbf{k} = \mathbf{0}$ term from the sum in (21). Then we obtain for the finite system in the large-n limit

$$\chi^{-1} = r_0 + 4u_0 n L^{-d} \chi + 4u_0 n L^{-d} \sum_{\mathbf{k} \neq \mathbf{0}} (\chi^{-1} + \mathbf{k}^2)^{-1}. \quad (27)$$

In the bulk limit χ_b^{-1} vanishes for $T \leq T_c$. Thus, together with (26), the bulk limit of (27) yields the square of the bulk order parameter M_b (per component) for $r_0 < r_{0c}$ and for $d > 2$

$$\lim_{V \to \infty} \lim_{n \to \infty} M^2 \equiv M_b^2 = \frac{r_{0c} - r_0}{4u_0 n} \quad (28)$$

in agreement with the known bulk result [19]. Equation (28) implies the bulk critical exponent $\beta = 1/2$ for general $d > 2$.

Finally we calculate the specific heat per unit volume and per component near T_c

$$C = -T_c^2 \frac{\partial^2}{\partial T^2} f = -a_0^2 \frac{\partial^2}{\partial r_0^2} f \tag{29}$$

where the constant $a_0 > 0$ is defined by

$$r_0 - r_{0c} = a_0 t, \; t = (T - T_c)/T_c. \tag{30}$$

In the large-n limit we obtain from (20, 29) for the finite system

$$C = \frac{a_0^2}{8u_0 n} \left\{ 1 + \left[\frac{4u_0 n}{L^d} \chi^2 + \frac{4u_0 n}{L^d} \sum_{\mathbf{k} \neq \mathbf{0}} (\chi^{-1} + \mathbf{k}^2)^{-2} \right]^{-1} \right\}^{-1}. \tag{31}$$

Here we have separated the $\mathbf{k} = \mathbf{0}$ term from the sum. For $T \geq T_c$ the bulk limit yields

$$C_b^+ = \frac{a_0^2}{8u_0 n} \left\{ 1 + \left[4u_0 n \int\limits_{\mathbf{k}} (\chi^{-1} + \mathbf{k}^2)^{-2} \right]^{-1} \right\}^{-1}. \tag{32}$$

Below T_c the $\mathbf{k} = \mathbf{0}$ term of (31) together with $\chi_b^{-1} = 0$ implies the temperature independent bulk result

$$C_b^- = \frac{a_0^2}{8u_0 n} \cdot \tag{33}$$

3 Finite-size effects in the φ^4 lattice model for n $\rightarrow \infty$

For comparison with the field-theoretic model we consider a lattice Hamiltonian $\hat{H}(\varphi_i)$ for n-component vectors φ_i with components $\varphi_{i\alpha}$, $-\infty \leq \varphi_{i\alpha} \leq \infty$, $\alpha = 1, 2, ..., n$ on the lattice points $\mathbf{x}_i$ of a simple-cubic lattice in a cube with volume $V = L^d$ and with periodic boundary conditions. We assume [23]

$$\hat{H}(\varphi_i) = \tilde{a}^d \left\{ \sum_i \left[\frac{\hat{r}_0}{2} \varphi_i^2 + \hat{u}_0 (\varphi_i^2)^2 \right] + \sum_{i,j} \frac{1}{2\tilde{a}^2} J_{ij} (\varphi_i - \varphi_j)^2 \right\} \tag{34}$$

where J_{ij} is a pair interaction and $\tilde{a}$ is the lattice spacing. The couplings J_{ij} are dimensionless quantities. The vectors φ_j have the Fourier representation

$$\varphi_j = \frac{1}{L^d} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}_j} \hat{\varphi}_{\mathbf{k}}. \tag{35}$$

In terms of the Fourier components

$$\hat{\varphi}_{\mathbf{k}} = \tilde{a}^d \sum_j e^{-i\mathbf{k}\cdot\mathbf{x}_j} \varphi_j \tag{36}$$

the Hamiltonian $\hat{H}$ reads

$$\hat{H} = L^{-d} \sum_{\mathbf{k}} \frac{1}{2} [\hat{r}_0 + 2\delta J(\mathbf{k})] \hat{\varphi}_{\mathbf{k}} \, \hat{\varphi}_{-\mathbf{k}} + \hat{u}_0 L^{-3d} \sum_{\mathbf{k}\mathbf{k}'\mathbf{k}''} (\hat{\varphi}_{\mathbf{k}} \, \hat{\varphi}_{\mathbf{k}'}) (\hat{\varphi}_{\mathbf{k}''} \, \hat{\varphi}_{-\mathbf{k}-\mathbf{k}'-\mathbf{k}''}) \tag{37}$$

where

$$\delta J(\mathbf{k}) = \frac{1}{\tilde{a}^2} [J(0) - J(\mathbf{k})] \tag{38}$$

with

$$J(\mathbf{k}) = (\tilde{a}/L)^d \sum_{i,j} J_{ij} e^{-i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)}. \tag{39}$$

The summation $\sum_{\mathbf{k}}$ runs over discrete $\mathbf{k}$ vectors with components $k_j = 2\pi m_j / L$, $m_j = 0, \pm 1, \pm 2, \cdots$, $j = 1, 2, \cdots, d$ in the range $-\Lambda \equiv -\pi/\tilde{a} \leq k_j < \pi/\tilde{a} \equiv \Lambda$. Comparison between (37) and (4) shows that the derivation of thermodynamic quantities for the finite lattice model is parallel to that of Section 2.

We consider the following quantities for the finite lattice: the Gibbs free energy per component and per unit volume

$$\hat{f} = -\frac{1}{nL^d} \ln \int \mathcal{D}\hat{\varphi} \exp(-\hat{H}), \tag{40}$$

the susceptibility (per component) at finite wave number

$$\hat{\chi}(\mathbf{k}) = \frac{\tilde{a}^{2d}}{nL^d} \sum_{i,j} \langle \varphi_i \, \varphi_j \rangle e^{-i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)}, \tag{41}$$

the order parameter

$$\hat{M} = \frac{\tilde{a}^d}{n^{1/2} L^d} \left[\left\langle \left(\sum_i \varphi_i \right)^2 \right\rangle \right]^{1/2} = L^{-d/2} \hat{\chi}^{1/2}, \tag{42}$$

where $\hat{\chi} \equiv \hat{\chi}(\mathbf{0})$ and the specific heat

$$\hat{C} = -T_c^2 \frac{\partial^2}{\partial T^2} \hat{f} = -\hat{a}_0^2 \frac{\partial^2}{\partial \hat{r}_0^2} \hat{f} \tag{43}$$

where

$$\hat{r}_0 - \hat{r}_{0c} = \hat{a}_0 t, \quad t = (T - T_c)/T_c. \tag{44}$$

In the limit $n \rightarrow \infty$ at fixed $\hat{u}_0 n$ the results for the quantities $\hat{f}, \hat{\chi}, \hat{M}, \hat{C}$, and $\hat{r}_{0c}$ can be obtained from those of Section 2 simply by replacing $r_0 \rightarrow \hat{r}_0$, $u_0 \rightarrow \hat{u}_0$, and $\mathbf{k}^2 \rightarrow 2\delta J(\mathbf{k})$. Thus

$$\hat{f} = \hat{f}_0 - \frac{(\hat{r}_0 - \hat{\chi}^{-1})^2}{16\hat{u}_0 n} + \frac{1}{2} L^{-d} \sum_{\mathbf{k}} \ln \left[\hat{\chi}^{-1} + 2\delta J(\mathbf{k}) \right], \tag{45}$$

$$\hat{\chi}^{-1} = \hat{r}_0 + 4\hat{u}_0 n L^{-d} \hat{\chi} + 4\hat{u}_0 n L^{-d} \sum_{\mathbf{k} \neq \mathbf{0}} \left[\hat{\chi}^{-1} + 2\delta J(\mathbf{k}) \right]^{-1}, \tag{46}$$

$$\hat{C} = \frac{\hat{a}_0^2}{8\hat{u}_0 n} \left\{ 1 + \left(\frac{4\hat{u}_0 n}{L^d} \hat{\chi}^2 + \frac{4\hat{u}_0 n}{L^d} \sum_{\mathbf{k} \neq \mathbf{0}} [\hat{\chi}^{-1} + 2\delta J(\mathbf{k})]^{-2} \right)^{-1} \right\}^{-1}, \tag{47}$$

$$\hat{r}_{0c} = -4\hat{u}_0 n \int\limits_{\mathbf{k}} \left[2\delta J(\mathbf{k}) \right]^{-2}. \tag{48}$$

The discussion of the bulk limits of these equations is parallel to that in Section 2. We assume a finite-range pair interaction such that its Fourier transform (39) has the small $\mathbf{k}$ behavior

$$\delta J(\mathbf{k}) = \frac{1}{2} J_0 \mathbf{k}^2 + \mathcal{O}(k_i^2 k_j^2) \tag{49}$$

with

$$J_0 = \frac{1}{d} (\tilde{a}/L)^d \sum_{i,j} \left(J_{ij}/\tilde{a}^2 \right) \left(\mathbf{x}_i - \mathbf{x}_j \right)^2 . \tag{50}$$

This implies that the bulk susceptibility above T_c

$$\hat{\chi}_b(\mathbf{k})^{-1} = \hat{\chi}_b^{-1} + 2\delta J(\mathbf{k}) \tag{51}$$

determines the square of the bulk correlation length of the lattice model above T_c

$$\hat{\xi}^2 = \hat{\chi}_b \left[\partial \hat{\chi}_b(\mathbf{k})^{-1} / \partial \mathbf{k}^2 \right]_{\mathbf{k}=\mathbf{0}} = J_0 \, \hat{\chi}_b . \tag{52}$$

4 Universal finite-size scaling functions for 2 < d < 4

In the following we derive the asymptotic (large L, small $|t|$) finite-size scaling functions of χ, M, C and of $\hat{\chi}, \hat{M}$, and $\hat{C}$ in the large-n limit for $2 < d < 4$. The scaling functions for the field-theoretic model (1) and the lattice model (34) will be verified to have the same universal form, apart from nonuniversal metric factors [24]. These factors turn out to depend on the strength J_0 of the pair interaction (50) and on the model parameters a_0, u_0 and $\hat{a}_0, \hat{u}_0$ but to be independent of the cutoff Λ and of the lattice spacing $\tilde{a}$.

4.1 Field-theoretic model

The first step is to rewrite χ, M and C as functions of $r_0 - r_{0c}, u_0 n$ and Λ. The second step is to perform a decomposition into bulk and finite-size contributions. The third step is to take the limit of large L and small $|r_0 - r_{0c}|$ at finite Λ. The resulting finite-size scaling functions will turn out to be independent of Λ for $2 < d < 4$. Alternatively, and more conveniently, we perform the third step by first letting $\Lambda \to \infty$ at fixed $r_0 - r_{0c} = a_0 t$. The asymptotic finite-size scaling functions are then obtained by dropping subleading terms in the limit of large L and large χ at fixed $\chi^{-1} L^2$.

Starting from (27), the first and second steps yield an implicit equation for $\chi(r_0 - r_{0c}, u_0 n, L, \Lambda, d)^{-1}$,

$$\chi^{-1} = r_0 - r_{0c} - \widetilde{\Delta}_1 + 4u_0 n \Big\{ \chi L^{-d} - \chi^{-1} \int_{\mathbf{k}} \left[\mathbf{k}^2 (\chi^{-1} + \mathbf{k}^2) \right]^{-1} \Big\} \tag{53}$$

where

$$\widetilde{\Delta}_1 = 4u_0 n \left[\int_{\mathbf{k}} (\chi^{-1} + \mathbf{k}^2)^{-1} - L^{-d} \sum_{\mathbf{k} \neq \mathbf{0}} (\chi^{-1} + \mathbf{k}^2)^{-1} \right] . \tag{54}$$

At fixed $r_0 - r_{0c}$, the limit $\Lambda \to \infty$ of (53) exists for $2 < d < 4$. Then we have

$$\lim_{\Lambda \to \infty} \int_{\mathbf{k}} [\mathbf{k}^2 (\chi^{-1} + \mathbf{k}^2)]^{-1} = A_d \, \chi^{\varepsilon/2} \, \varepsilon^{-1} \tag{55}$$

with $\varepsilon = 4 - d$,

$$A_d = \Gamma(3 - d/2) 2^{2-d} \pi^{-d/2} (d-2)^{-1} \tag{56}$$

with $A_3 = (4\pi)^{-1}$, and

$$\lim_{\Lambda \to \infty} \widetilde{\Delta}_1 = 4u_0 n L^{2-d} \, I_1(\chi^{-1} L^2), \tag{57}$$

$$I_1(x) = -(2\pi)^{-2} \int_0^\infty dy \, e^{-(xy/4\pi^2)} \left[K(y)^d - (\pi/y)^{d/2} - 1 \right], \tag{58}$$

$$K(y) = \sum_{m=-\infty}^{\infty} e^{-ym^2}. \tag{59}$$

Multiplication of (53) by L^{d-2} yields for $\Lambda \to \infty$ (at fixed $a_0 t$)

$$\left(\chi^{-1} L^2 \right) L^{d-4} = a_0 t L^{d-2} + 4u_0 n [\chi L^{-2} - A_d \varepsilon^{-1} \left(\chi L^{-2} \right)^{(2-d)/2} - I_1 \left(\chi^{-1} L^2 \right)]. \tag{60}$$

Taking the limit of large L and large χ at fixed $\chi^{-1} L^2$ eliminates the non-scaling term on the l.h.s. of (60) and determines the dimensionless asymptotic scaling function $P_\chi \left(t (L/\xi_0)^{1/\nu} \right)$,

$$\chi(t, L) = L^{\gamma/\nu} \, P_\chi \left(t (L/\xi_0)^{1/\nu} \right), \tag{61}$$

according to

$$0 = t (L/\xi_0)^{1/\nu} - (P_\chi)^{-1/\gamma} + \varepsilon A_d^{-1} \left[P_\chi - I_1 (P_\chi^{-1}) \right] \tag{62}$$

with the critical exponents $\nu = (d-2)^{-1}$ and $\gamma = 2/(d-2)$ for $2 < d < 4$ and with the reference length

$$\xi_0 = \left(\frac{4u_0 n A_d}{\varepsilon a_0} \right)^{1/(d-2)} . \tag{63}$$

Using (23) it is straightforward to show by means of (61, 62) that ξ_0 is the amplitude of the bulk correlation length $\xi \sim \xi_0 t^{-\nu}$ above T_c. We see that the nonuniversal model parameters a_0 und u_0 enter only *via* ξ_0.

The dimensionless finite-size scaling function $P_M(t(L/\xi_0)^{1/\nu})$ of

$$M = L^{\beta/\nu}\, P_M(t(L/\xi_0)^{1/\nu}) \tag{64}$$

is immediately obtained from (26, 61) as

$$P_M\left(t(L/\xi_0)^{1/\nu}\right) = \left[P_\chi\left(t(L/\xi_0)^{1/\nu}\right)\right]^{1/2}. \tag{65}$$

Similar calculations for the specific heat yield, starting from (31),

$$C = \frac{a_0^2}{8u_0 n}\{1 + [4u_0 n L^{-d}\,\chi^2 - \widetilde{\Delta}_2 + 4u_0 n \int\limits_{\mathbf{k}} (\chi^{-1} + \mathbf{k}^2)^{-2}\Big]^{-1}\Big\}^{-1}, \tag{66}$$

$$\widetilde{\Delta}_2 = 4u_0 n\Big[\int\limits_{\mathbf{k}} (\chi^{-1} + \mathbf{k}^2)^{-2} - L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}} (\chi^{-1} + \mathbf{k}^2)^{-2}\Big], \tag{67}$$

which determines $C(r_0 - r_{0c}, u_0 n, L, \Lambda, d)$. In the limit $\Lambda \to \infty$ at fixed $r_0 - r_{0c}$ we obtain for $0 < \varepsilon < 2$

$$\lim_{\Lambda\to\infty} \int\limits_{\mathbf{k}} (\chi^{-1} + \mathbf{k}^2)^{-2} = A_d\,\chi^{\varepsilon/2}\,\varepsilon^{-1}(1 - \varepsilon/2), \tag{68}$$

$$\lim_{\Lambda\to\infty} \widetilde{\Delta}_2 = 4u_0 n L^{4-d}\, I_2(\chi^{-1}L^2), \tag{69}$$

$$I_2(x) = -(2\pi)^{-4}\int_0^\infty dy\, y\, e^{-(xy/4\pi^2)}\left[K(y)^d - (\pi/y)^{d/2} - 1\right], \tag{70}$$

$$C = \frac{a_0^2}{8u_0 n}\Big\{1 + (4u_0 n)^{-1}L^{d-4} \times \left[P_\chi^2 + \frac{A_d}{\varepsilon}\left(1 - \frac{\varepsilon}{2}\right) P_\chi^{\varepsilon/2} - I_2\left(P_\chi^{-1}\right)\right]^{-1}\Big\}^{-1}. \tag{71}$$

In the limit of large L at fixed $\chi^{-1}L^2$ the resulting finite-size scaling function $P_C(t(L/\xi_0)^{1/\nu})$ of the specific heat

$$C(t, L) - C(0, \infty) = L^{\alpha/\nu} P_C\left(t(L/\xi_0)^{1/\nu}\right) \tag{72}$$

can be expressed in terms of $P_\chi\left(t(L/\xi_0)^{1/\nu}\right)$ according to

$$P_C(t(L/\xi_0)^{1/\nu}) = -A_C[P_\chi^2 + \frac{A_d}{\varepsilon}(1 - \frac{\varepsilon}{2})P_\chi^{\varepsilon/2} - I_2(P_\chi^{-1})]^{-1}, \tag{73}$$

with the nonuniversal factor

$$A_C = \frac{a_0^2}{32(u_0 n)^2} \tag{74}$$

and the critical exponent $\alpha = (d-4)/(d-2)$ for $2 < d < 4$.

4.2 Lattice model

For the case of the lattice Hamiltonian the scaling limit of large L and small $|t|$ will be performed at fixed lattice spacing $\tilde{a}$. For the finite-range pair interaction (39) the form of $J(\mathbf{k})$ at finite $\mathbf{k}$ does not affect the asymptotic scaling region for $2 < d < 4$. The finite-size scaling functions $\hat{P}_\chi$, $\hat{P}_M$ and $\hat{P}_C$ are modified (compared to P_χ, P_M, P_C) only through nonuniversal metric factors that are independent of Λ and $\tilde{a}$.

For $\hat{\chi}$, these factors arise in the limit of large $\hat{\chi}$ from

$$\int\limits_{\mathbf{k}} \Big\{2\delta J(\mathbf{k})\big[\hat{\chi}^{-1} + 2\delta J(\mathbf{k})\big]\Big\}^{-1} \sim J_0^{-d/2} A_d\,\hat{\chi}^{\varepsilon/2}\;\varepsilon^{-1} \tag{75}$$

and, in the limit of large $\hat{\chi}$ and large L at fixed $\hat{\chi}^{-1}L^2$, from

$$\int\limits_{\mathbf{k}} \left[\hat{\chi}^{-1} + 2\delta J(\mathbf{k})\right]^{-1} - L^{-d}\sum_{\mathbf{k}\neq 0}\left[\hat{\chi}^{-1} + 2\delta J(\mathbf{k})\right]^{-1} \sim J_0^{-1}L^{2-d}\, I_1\left(J_0^{-1}\hat{\chi}^{-1}L^2\right). \tag{76}$$

For $\hat{P}_\chi = \hat{\chi}L^{-\gamma/\nu}$ this leads to

$$0 = t(L/\hat{\xi}_0)^{1/\nu} - (J_0\hat{P}_\chi)^{-1/\gamma} + \varepsilon A_d^{-1}[J_0\hat{P}_\chi - I_1(J_0^{-1}\hat{P}_\chi^{-1})] \tag{77}$$

where now $\hat{\xi}_0$ is the reference length of the lattice model,

$$\hat{\xi}_0 = \left[\frac{4\hat{u}_0 n A_d}{\varepsilon\hat{a}_0 J_0}\right]^{1/(d-2)}. \tag{78}$$

Using (52) it is straightforward to show by means of (77) that $\hat{\xi}_0$ is indeed the amplitude of the bulk correlation length $\hat{\xi} \sim \hat{\xi}_0 t^{-\nu}$ of the lattice model above T_c. Thus we define $\hat{P}_\chi$ with the appropriate scaling variable as

$$\hat{\chi}(t, L) = L^{\gamma/\nu}\hat{P}_\chi\left(t(L/\hat{\xi}_0)^{1/\nu}\right). \tag{79}$$

Comparison of (77) with (62) implies the relation

$$J_0\,\hat{P}_\chi\left(t(L/\hat{\xi}_0)^{1/\nu}\right) = P_\chi\left(t(L/\hat{\xi}_0)^{1/\nu}\right) = P_\chi\left((\xi_0/\hat{\xi}_0)^{1/\nu} t(L/\xi_0)^{1/\nu}\right), \tag{80}$$

i.e., $\hat{P}_\chi$ and P_χ are the same universal functions up to factors J_0 and $(\xi_0/\hat{\xi}_0)^{1/\nu}$. These factors are independent of Λ and $\tilde{a}$. Similarly we obtain for $\hat{M} = L^{\beta/\nu}\hat{P}_M$ the relation $\hat{P}_M = (\hat{P}_\chi)^{1/2}$ and

$$J_0^{1/2}\,\hat{P}_M\left(t(L/\hat{\xi}_0)^{1/\nu}\right) = P_M\left(t(L/\hat{\xi}_0)^{1/\nu}\right) = P_M\left((\xi_0/\hat{\xi}_0)^{1/\nu} t(L/\xi_0)^{1/\nu}\right). \tag{81}$$

Finally we present the asymptotic scaling function $\hat{P}_C$ of the specific heat

$$\hat{C}(t,L) - \hat{C}(0,\infty) = L^{\alpha/\nu}\hat{P}_C\left(t(L/\hat{\xi}_0)^{1/\nu}\right) \quad (82)$$

of the lattice model. Like $P_C, \hat{P}_C$ can be expressed in terms of $\hat{P}_\chi\left(t(L/\hat{\xi}_0)^{1/\nu}\right)$ according to

$$\hat{P}_C\left(t(L/\hat{\xi}_0)^{1/\nu}\right) = -\hat{A}_C\left[(J_0\hat{P}_\chi)^2 + \frac{A_d}{\varepsilon}(1-\frac{\varepsilon}{2})(J_0\hat{P}_\chi)^{\varepsilon/2} - I_2\left(J_0^{-1}\hat{P}_\chi^{-1}\right)\right]^{-1} \quad (83)$$

with the nonuniversal factor

$$\hat{A}_C = \frac{(\hat{a}_0 J_0)^2}{32(\hat{u}_0 n)^2}\,. \quad (84)$$

Comparison of equations (83, 84) with equations (73, 74, 80) implies the relation

$$\frac{A_C}{\hat{A}_C}\,\hat{P}_C\left(t(L/\hat{\xi}_0)^{1/\nu}\right) = P_C\left(t(L/\hat{\xi}_0)\right) = P_C\left((\xi_0/\hat{\xi}_0)^{1/\nu}t(L/\xi_0)^{1/\nu}\right). \quad (85)$$

In summary, the expected universality of all finite-size scaling functions is confirmed for $2 < d < 4$, up to the factors $A_C/\hat{A}_C$ and J_0 which are independent of Λ and $\tilde{a}$. In all cases the amplitude of the bulk correlation length appears as the natural reference length, and the same factor $(\xi_0/\hat{\xi}_0)^{1/\nu}$ appears in the scaling argument of both P_χ, equation (80), and P_C, equation (85). The issue of universality and metric factors [3,24] will be further discussed elsewhere [25].

As a general remark we note that for the finite system the critical exponents appearing in the finite-size scaling relations are meaningful in the entire range of validity of these scaling forms, *i.e.*, also below T_c, even if in the bulk limit below T_c the notion of α and γ may be considered as problematic for $n\to\infty$ (since C_b^- is temperature independent and no finite χ_b exists below T_c).

5 Finite-size and lattice effects for d > 4

As pointed out recently [13] there exist significant differences between the leading finite-size effects on the field-theoretic version χ and on the lattice version $\hat{\chi}$ of the susceptibility at T_c for $d > 4$. In the following we further extend this analysis. Throughout this section it will be necessary to keep Λ finite.

5.1 Susceptibility and order parameter for d > 4

First we consider the field-theoretic model with H, equation (1). Adding and subtracting $4u_0 n\, L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}\mathbf{k}^{-2}$ in (27) and rewriting $r_0 = r_0 - r_{0c} - 4u_0 n\int_{\mathbf{k}}\mathbf{k}^{-2}$ yields

$$\chi^{-1} = \delta r_0 + 4u_0 n L^{-d}\chi - \chi^{-1}S \quad (86)$$

or

$$\chi^{-1} = \frac{\delta r_0 + \sqrt{(\delta r_0)^2 + 16u_0 n L^{-d}(1+S)}}{2(1+S)} \quad (87)$$

where

$$\delta r_0 = r_0 - r_{0c} - \Delta, \quad (88)$$

$$S = 4u_0 n L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}\left[\mathbf{k}^2(\chi^{-1}+\mathbf{k}^2)\right]^{-1}, \quad (89)$$

$$\Delta = 4u_0 n\left[\int_{\mathbf{k}}\mathbf{k}^{-2} - L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}\mathbf{k}^{-2}\right]. \quad (90)$$

For the lattice Hamiltonian $\hat{H}$ the corresponding result is

$$\hat{\chi}^{-1} = \frac{\delta\hat{r}_0 + \sqrt{(\delta\hat{r}_0)^2 + 16\hat{u}_0 n L^{-d}(1+\hat{S})}}{2(1+\hat{S})} \quad (91)$$

where

$$\delta\hat{r}_0 = \hat{r}_0 - \hat{r}_{0c} - \hat{\Delta}, \quad (92)$$

$$\hat{S} = 4\hat{u}_0 n L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}\left\{2\,\delta J(\mathbf{k})\left[\hat{\chi}^{-1} + 2\,\delta J(\mathbf{k})\right]\right\}^{-1}, \quad (93)$$

$$\hat{\Delta} = 4\hat{u}_0 n\left[\int_{\mathbf{k}}\frac{1}{2\,\delta J(\mathbf{k})} - L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}\frac{1}{2\,\delta J(\mathbf{k})}\right]. \quad (94)$$

The lowest-mode approach [17] neglects the contributions of the $\mathbf{k}\neq\mathbf{0}$ modes, *i.e.*, it corresponds to the approximation $S = 0, \Delta = 0$, and $\hat{S} = 0$, $\hat{\Delta} = 0$. The large-L behavior of Δ for $d > 2$ is nontrivial,

$$\Delta \sim 4u_0 n\Lambda^{d-2}\Big[a_1(d)(\Lambda L)^{-2} + a_2(d)(\Lambda L)^{2-d} + \mathcal{O}((\Lambda L)^{-4})\Big] \quad (95)$$

(see Appendix). The corresponding quantity of the lattice model has the simpler large-L behavior for $d > 2$

$$\hat{\Delta} \sim 4\hat{u}_0 n J_0^{-1}a_2(d)L^{2-d}, \quad (96)$$

apart from more rapidly vanishing terms. The coefficients $a_i(d) > 0$ are given in Appendix. We have confirmed the results (95, 96) by numerical evaluation of equations (90, 94) [13].

We point out that the difference between Δ and $\hat{\Delta}$ has crucial consequences for the issue of universality and finite-size scaling for $d > 4$ to be discussed in the subsequent section. Most important is the difference between Δ and $\hat{\Delta}$ with regard to the large L behavior. Equations (95, 96) imply the large-L behavior at T_c for $d > 4$

$$\chi_c \sim \frac{L^d\Delta}{4u_0 n} \sim a_1(d)\Lambda^{d-4}L^{d-2} \quad (97)$$

and

$$\hat{\chi}_c \sim (4\hat{u}_0 n)^{-1/2}(1+\hat{S}_c^b)^{1/2}L^{d/2} \quad (98)$$

with $\hat{S}_c^b = 4\hat{u}_0 n \int_{\mathbf{k}} [2\ \delta J(\mathbf{k})]^{-2}$ whereas the lowest-mode approach yields

$$\chi_{0c} = (4u_0 n)^{-1/2} L^{d/2} \tag{99}$$

and

$$\hat{\chi}_{0c} = (4\hat{u}_0 n)^{-1/2} L^{d/2}. \tag{100}$$

Some of the implications of these results have been discussed in reference [13].

Here we proceed to the case $T > T_c$. For small but finite $t > 0$ we obtain the bulk and the leading finite-size terms for $d > 4$ in the large-L limit

$$\chi^{-1} = (1 + S_c^b)^{-1} \left(a_0 t - 4u_0 n \Lambda^{d-4} a_1(d)\ L^{-2} \right) \tag{101}$$

$$\hat{\chi}^{-1} = (1 + \hat{S}_c^b)^{-1} \left(\hat{a}_0 t - 4\hat{u}_0 n J_0^{-1} [I_1(\hat{x}) - \hat{x}^{-1}]\ L^{2-d} \right) \tag{102}$$

with $S_c^b = 4u_0 n \int_{\mathbf{k}} \mathbf{k}^{-4}$ and $\hat{x} = tL^2 \hat{\xi}_0^{-2}$. We see that the leading finite-size terms above T_c have different power laws for the field-theoretic and the lattice model. For comparison we consider the corresponding results of the lowest-mode approach for $t > 0$ and large L,

$$\chi_0^{-1} = a_0 t + 4u_0 n\ L^{-d}/(a_0 t), \tag{103}$$

$$\hat{\chi}_0^{-1} = \hat{a}_0 t + 4\hat{u}_0 n\ L^{-d}/(\hat{a}_0 t). \tag{104}$$

We conclude that the lowest-mode approach fails above T_c with regard to the leading finite-size terms for both the field-theoretic and the lattice model.

On the basis of the relations (25, 42), analogous results are obtained for the order parameter for $d > 4$, *e.g.*, at T_c for the field-theoretic model

$$M_c^2 = L^{-d} \chi_c \sim a_1(d) \Lambda^{d-4} L^{-2} \tag{105}$$

and for the lattice model

$$\hat{M}_c^2 = L^{-d} \hat{\chi}_c \sim (4\hat{u}_0 n)^{-1/2} (1 + \hat{S}_c^b)^{1/2} L^{-d/2}, \tag{106}$$

whereas the lowest-mode approach yields

$$M_{0c}^2 = (4u_0 n)^{-1/2} L^{-d/2} \tag{107}$$

and

$$\hat{M}_{0c}^2 = (4\hat{u}_0 n)^{-1/2} L^{-d/2}. \tag{108}$$

We note that the previous arguments [17] in support of the asymptotic correctness of the lowest-mode approach for $d > 4$ are not sufficiently compelling and complete since they are focused only on the rescaling of individual terms at lowest non-zero $\mathbf{k}$ (see Eq. (3.17b) of Ref. [17] and the preceding equation) without calculating the sum of these terms. Also in the recent more detailed exposition [19] no argument is presented that indicates why it should be unnecessary to carry out the summation in equation (36.33) of reference [19] in addition to the rescaling of individual terms. We claim that this summation is crucial, for large L, as demonstrated in Appendix for the quantity Δ.

5.2 Specific heat at T_c for $d > 4$

The expressions for the specific heat of the finite system at T_c are obtained from (31, 47) as

$$C_c(L) = \frac{a_0^2}{8u_0 n} \Big\{ 1\ + \Big[\frac{4u_0 n}{L^d}\ \chi_c^2 + \frac{4u_0 n}{L^d} \sum_{\mathbf{k}\neq\mathbf{0}} (\chi_c^{-1} + \mathbf{k}^2)^{-2} \Big]^{-1} \Big\}^{-1} \tag{109}$$

and

$$\hat{C}_c(L) = \frac{\hat{a}_0^2}{8\hat{u}_0 n} \Big\{ 1 + \Big(\frac{4\hat{u}_0 n}{L^d} \hat{\chi}_c^2 + \frac{4\hat{u}_0 n}{L^d} \sum_{\mathbf{k}\neq\mathbf{0}} \big[\hat{\chi}_c^{-1} + 2\delta J(\mathbf{k}) \big]^{-2} \Big)^{-1} \Big\}^{-1}, \tag{110}$$

for the field-theoretic and the lattice model, respectively. In the bulk limit the sums $L^{-d} \sum_{\mathbf{k}} \neq \mathbf{0}$ in both (109, 110) become finite integrals for $d > 4$. The basic difference between $C_c(L)$ and $\hat{C}_c(L)$ for large L arises from the $\mathbf{k} = \mathbf{0}$ terms $4u_0 n\ L^{-d} \chi_c^2$ and $4\hat{u}_0 n\ L^{-d} \hat{\chi}_c^2$. According to (97, 98), the field-theoretic term proportional to $L^{-d} \chi_c^2$ diverges as L^{d-4} whereas the lattice term proportional to $L^{-d} \hat{\chi}_c^2$ remains finite for $L \to \infty$. This implies different bulk values and different finite-size effects at T_c. The finite bulk values are for $d > 4$

$$\lim_{L\to\infty} C_c(L) \equiv C_c^b = \frac{a_0^2}{8u_0 n} \tag{111}$$

and

$$\lim_{L\to\infty} \hat{C}_c(L) \equiv \hat{C}_c^b = \frac{\hat{a}_0^2}{8\hat{u}_0 n} \Big\{ 1 + \Big[1 + 2\hat{S}_c^b \Big]^{-1} \Big\}^{-1}. \tag{112}$$

We note that $\lim_{t\to+0} \Big[\lim_{L\to\infty} \hat{C}(t, L) \Big] \neq \hat{C}_c^b$. The leading finite-size effects at T_c are for $d > 4$

$$C_c^b - C_c(L) \sim C_c^b \left[4u_0 n\ \Lambda^{d-4} a_1(d)^2 \right]^{-1} (\Lambda L)^{4-d} \tag{113}$$

and

$$\hat{C}_c^b - \hat{C}_c(L) \sim -\hat{C}_c^b \frac{(4\hat{u}_0 n\ \tilde{a}^{4-d})^{1/2}\ a_2(d)}{4J_0\ (1 + \hat{S}_c^b)^{3/2}}\ (L/\tilde{a})^{(4-d)/2}. \tag{114}$$

We see that the field-theoretic Hamiltonian H and the lattice Hamiltonian $\hat{H}$ yield significantly different finite-size effects on the specific heat at T_c for $d > 4$. A more complete study of C and $\hat{C}$ is given elsewhere [25].

We compare these results with the specific heat C_0 and $\hat{C}_0$ obtained within the lowest-mode approach. Neglecting the $\mathbf{k} \neq \mathbf{0}$ terms in (31, 47) we obtain the lowest-mode results at T_c for the finite system

$$C_{0c} = \frac{a_0^2}{8u_0 n} \left\{ 1 + \frac{L^d}{4u_0 n} \chi_{0c}^{-2} \right\}^{-1} \tag{115}$$

and

$$\hat{C}_{0c} = \frac{\hat{a}_0^2}{8\hat{u}_0 n} \left\{ 1 + \frac{L^d}{4\hat{u}_0 n} \hat{\chi}_{0c}^{-2} \right\}^{-1} \tag{116}$$

for $d > 4$. Together with (99, 100) this yields the L-independent constants for the finite systems

$$C_{0c} = \frac{a_0^2}{16 u_0 n},\ \hat{C}_{0c} = \frac{\hat{a}_0^2}{16\hat{u}_0 n}\,\cdot \tag{117}$$

Thus the lowest-mode approach does not capture any finite-size effect on the specific heat at T_c for $d > 4$, even for small systems where finite-size effects become large. We do not consider this to be an acceptable approximation in view of the leading finite-size effects determined by the results in (113, 114).

6 Finite-size scaling functions for d > 4

In the following we shall show that for large L and small $|t|$ the susceptibilities χ and $\hat{\chi}$ of both the φ^4 field theory and the φ^4 lattice model do not have the usual universal scaling forms of (61, 79) for $d > 4$. This was to be expected from previous work [5,6]. As a new result we find that, in the large-n limit at fixed $u_0 n$ and $\hat{u}_0 n$, χ and $\hat{\chi}$ attain the generalized finite-size scaling forms

$$\chi = L^{\gamma/\nu} P_\chi \Big(t (L/\xi_0)^{1/\nu},\, c_0 u_0 n L^{4-d} \Big) \tag{118}$$

and

$$\hat{\chi} = L^{\gamma/\nu} \hat{P}_\chi \Big(t (L/\hat{\xi}_0)^{1/\nu},\, \hat{c}_0 \hat{u}_0 n L^{4-d} \Big) \tag{119}$$

for $d > 4$ with a *nonuniversal* scaling function P_χ. Here we shall determine the exact scaling functions P_χ and $\hat{P}_\chi$ which turn out to differ significantly from each other, not only through metric factors. The structure of (118) was proposed earlier [15] for $d > 4$ on the basis of renormalization-group arguments (see Eq. (2.52) of Ref. [10]) but no specific form for the scaling function was given. In particular, the possibility of different structures of the scaling functions P_χ and $\hat{P}_\chi$ was not anticipated. In fact, it was suggested [10] in the context of the field-theoretic Hamiltonian (1) that a *universal* scaling function exists for $d > 4$ (see Eq. (2.57) of Ref. [10]).

For the case of the susceptibility of a modified version of the mean spherical model on a lattice [6], we have found that the result presented in equation (114) of reference [6] and equation (47) of reference [7] disagrees with the scaling structure of (119) as will be shown in Section 6.3 below. This disagreement has previously not been noticed in the literature.

6.1 Field-theoretic model

For large L and small $|t|$ we obtain the asymptotic form of χ^{-1} from (87, 95) for $d > 4$ as

$$\chi^{-1} = L^{-2} \frac{L^2\delta r + \sqrt{(L^2\delta r)^2 + 16 u_0 n L^{4-d}(1+S_c^b)}}{2(1+S_c^b)} \tag{120}$$

where

$$S_c^b = 4 u_0 n \int_{\mathbf{k}} \mathbf{k}^{-4} = 4\bar{u} n c_d \tag{121}$$

is a dimensionless constant and

$$L^2 \delta r = a_0 t L^2 - 4\bar{u} n\, a_1(d) \tag{122}$$

contains the temperature dependence. In S_c^b and $L^2\delta r$ the coupling u_0 appears in combination with the factor Λ^{d-4} which leads in a natural way to the dimensionless cutoff-dependent parameter

$$\bar{u} = u_0 \Lambda^{d-4}. \tag{123}$$

This is not the case for the coupling u_0 appearing in the $\mathbf{k} = \mathbf{0}$ term $16 u_0 n L^{4-d}$ in (120) which requires to combine this u_0 with the factor L^{4-d}. The coupling $u_0 L^{4-d}$ plays a role that differs fundamentally from that of $\bar{u}$ in (121, 122). This is seen from the singular dependence of χ on this u_0

$$\chi = L^2 \frac{|\delta r|}{4 u_0 n L^{4-d}} \left[1 + \mathcal{O}(u_0 n L^{4-d}) \right], \tag{124}$$

as obtained from (120) in the large L limit at finite negative $\delta r < 0$. Clearly this large-L limit reveals this u_0 to be the "dangerous irrelevant variable" anticipated earlier [14] which for the finite system ought to be combined with the factor L^{4-d} to yield the appropriate dimensionless scaling variable $u_0 L^{4-d}$ in the finite-size scaling theory [15]. This implies that (120) can be written in the finite-size scaling form

$$\chi = L^{\gamma/\nu}\, P_\chi \Big(t (L/\xi_0)^{1/\nu},\, (L/l_0)^{4-d} \Big) \tag{125}$$

for $d > 4$ with $\gamma = 1, \nu = 1/2$ and with the scaling function

$$P_\chi(x, y) = 2 \left\{ \delta(x) + \sqrt{[\delta(x)]^2 + 4y} \right\}^{-1}, \tag{126}$$

$$\delta(x) = x - (1 + S_c^b)^{-1} 4\bar{u} n a_1(d). \tag{127}$$

Here we have introduced the reference length

$$l_0 = \left(\frac{4 u_0 n}{1 + S_c^b} \right)^{1/(d-4)} \tag{128}$$

which becomes relevant above four dimensions. In addition we have used the amplitude

$$\xi_0 = \left[(1 + S_c^b)/a_0 \right]^{1/2} \tag{129}$$

of the bulk correlation length $\xi \sim \xi_0 t^{-\nu}$ above T_c which follows from (120, 23) for $d > 4$. Similarly, the order parameter has a scaling form for $d > 4$

$$M = L^{[(\gamma/\nu)-d]/2}\, P_M\Big(t(L/\xi_0)^{1/\nu}, (L/l_0)^{4-d}\Big) \tag{130}$$

with

$$P_M(x,y) = \Big[P_\chi(x,y)\Big]^{1/2} \tag{131}$$

because of (26).

One basic difference between the finite-size scaling functions for $2 < d < 4$ and for $d > 4$ is that the former are universal whereas the latter are nonuniversal. This nonuniversal structure arises from the L-independent dimensionless parameter $\bar{u}$, equation (123). This parameter causes a non-universal cutoff-dependent shift of the scaling variable x in the last term of $\delta(x)$, equation (127). Although the parameter $\bar{u}$ does not enter P_χ in a singular way there is no smallness argument that would permit one to expand $P_\chi(x,y)$ with respect to $\bar{u}$ and to retain only the part of P_χ at $\bar{u} = 0$. In the terminology of the renormalization group (RG), this parameter $\bar{u}$ does not have a RG flow and does not approach a "Gaussian fixed point", unlike the dangerous irrelevant coupling $u_0 L^{4-d}$. Thus the *asymptotic* (large L, small $|t|$) scaling function $P_\chi(x,y)$ is truely nonuniversal for $d > 4$.

In retrospect we now see that χ_c and M_c^2 in (97, 105) have not yet been represented in a scaling form in the sense of (118, 131). Application of the scaling functions P_χ, equation (126), and P_M, equation (131), to the case $x = 0$ reproduces the leading power laws of χ_c and M_c^2 in the appropriate scaling forms

$$\chi_c \sim \frac{a_1(d)\bar{u}}{u_0 L^{4-d}} L^{\gamma/\nu} \tag{132}$$

and

$$M_c^2 \sim \frac{a_1(d)\bar{u}}{u_0 L^{4-d}}\, L^{(\gamma/\nu)-d}. \tag{133}$$

6.2 Lattice model

From the lattice version of (53, 54) and from (76) we get the asymptotic (large L, small $|t|$) form of $\hat{\chi}^{-1}$ for $d > 4$ as

$$\hat{\chi}^{-1} = L^{-2}\, \frac{L^2\delta\hat{r} + \sqrt{(L^2\delta\hat{r})^2 + 16\hat{u}_0 n L^{4-d}(1+\hat{S}_c^b)}}{2(1+\hat{S}_c^b)} \tag{134}$$

where

$$\hat{S}_c^b = 4\hat{u}_0 n \int\limits_{\mathbf{k}} \left[2\delta J(\mathbf{k})\right]^{-2} = 4\bar{\hat{u}} n\hat{c} \tag{135}$$

is a dimensionless constant and

$$L^2\delta\hat{r} = \hat{a}_0 t L^2 - 4\hat{u}_0 n L^{4-d} J_0^{-1} I_1(J_0^{-1}\hat{\chi}^{-1}L^2) \tag{136}$$

contains the temperature dependence. We note that now the cutoff (lattice-spacing) dependent dimensionless parameter

$$\bar{\hat{u}} = \hat{u}_0 \tilde{a}^{4-d} \tag{137}$$

enters only $\hat{S}_c^b$, equation (135), but not $\delta\hat{r}$. In $\delta\hat{r}$ the same combination $\hat{u}_0 n L^{4-d}$ appears as in the zero-mode term $16\hat{u}_0 n L^{4-d}$ in (134). It is only the latter which is of a "dangerous irrelevant" character. The $4\hat{u}_0 n L^{4-d}$ term in (136) originates from the $\mathbf{k} \neq \mathbf{0}$ modes and enters $\hat{\chi}^{-1}$ in a non-singular way. At first sight, since it vanishes in the large-L limit for $d > 4$, this term appears to be a negligible correction that should not be retained in the asymptotic expression for $\hat{\chi}^{-1}$. This conclusion is, however, incorrect because this term contributes to the *leading* finite-size term for $T > T_c$ as presented in (102) of the preceding Section. If it were neglected the "dangerous" term $16\hat{u}_0 n L^{4-d}$ – which must of course be retained in any case – would become the leading finite-size term above T_c (corresponding to the lowest-mode approximation). This would simply be incorrect. Thus the second term on the r.h.s. of (136) *must be included* as a generic part of the asymptotic scaling function $\hat{P}_\chi$. From (134–137) we then obtain

$$\hat{\chi} = L^{\gamma/\nu}\, \hat{P}_\chi\Big(t(L/\hat{\xi}_0)^{1/\nu},\ (L/\hat{l}_0)^{4-d}\Big), \tag{138}$$

$$\hat{P}_\chi(\hat{x},\hat{y}) = 2J_0^{-1}\left\{\hat{\delta}(\hat{x},\hat{y}) + \sqrt{\Big[\hat{\delta}(\hat{x},\hat{y})\Big]^2 + 4\hat{y}}\right\}^{-1}, \tag{139}$$

$$\hat{\delta}(\hat{x},\hat{y}) = \hat{x} - I_1(J_0^{-1}\hat{P}_\chi^{-1})\hat{y}. \tag{140}$$

Here we have introduced the reference length of the lattice model

$$\hat{l}_0 = \left[\frac{4\hat{u}_0 n}{J_0^2(1+\hat{S}_c^b)}\right]^{1/(d-4)} \tag{141}$$

which becomes relevant above four dimensions. In addition we have used the amplitude

$$\hat{\xi}_0 = \Big[J_0(1+\hat{S}_c^b)/\hat{a}_0\Big]^{1/2} \tag{142}$$

of the bulk correlation length $\hat{\xi} \sim \hat{\xi}_0 t^{-\nu}$ above T_c which follows from (134, 52).

We see that $\hat{P}_\chi$ differs from P_χ, equation (126), not only by a metric (overall) factor J_0 (which would correspond to the case $2 < d < 4$) but exhibits a different structure. Now the quantity $\hat{\delta}(\hat{x},\hat{y})$ which plays the role of a scaled temperature variable contains an $\hat{y}$-dependent shift, in contrast to the *constant* shift of $\delta(x)$, equation (127). It is this different structure which leads to the different power laws of χ_c and $\hat{\chi}_c$ presented in reference [13] and in the preceding section. The origin of this structural difference is the different large-L behavior of Δ and $\hat{\Delta}$, equations (95, 96).

The same conclusions hold for the order parameters M and

$$\hat{M} = L^{[(\gamma/\nu)-d]/2} \hat{P}_M\Big(t(L/\hat{\xi}_0)^{1/\nu}, (L/\hat{l}_0)^{4-d}\Big). \quad (143)$$

The scaling function of the latter is

$$\hat{P}_M(\hat{x},\hat{y}) = \Big[\hat{P}_\chi(\hat{x},\hat{y})\Big]^{1/2} \quad (144)$$

according to (42).

We conclude that although the field-theoretic φ^4 model and φ^4 lattice model exhibit the same kind of bulk (mean field) critical behavior for $d > 4$ their finite-size scaling functions differ significantly.

For comparison we finally present the scaling functions $P_{0\chi}$ and $\hat{P}_{0\chi}$ of the lowest-mode approach,

$$P_{0\chi}(x_0,y_0) = 2\Big\{x_0 + \sqrt{x_0^2 + 4y_0}\Big\}^{-1}, \quad (145)$$

$$x_0 = t(La_0^{1/2})^{1/\nu},\ y_0 = 4u_0 n L^{4-d}, \quad (146)$$

and

$$\hat{P}_{0\chi}(\hat{x}_0,\hat{y}_0) = 2J_0^{-1}\Big\{\hat{x}_0 + \sqrt{\hat{x}_0^2 + 4\hat{y}_0}\Big\}^{-1}, \quad (147)$$

$$\hat{x}_0 = t(L\hat{a}_0^{1/2}J_0^{-1/2})^{1/\nu},\ \hat{y}_0 = 4\hat{u}_0 n L^{4-d} J_0^{-2}. \quad (148)$$

We see that these functions appear to have the same universal form for both the field-theoretic and the lattice model, in disagreement with P_χ and $\hat{P}_\chi$, equations (126, 139).

6.3 Comparison with previous results for d > 4

In the following we comment on the previous exact solutions of the n-vector model for $n \to \infty$ [5] and of the mean spherical model [6,7] on finite lattices. These solutions do not explicitly contain a variable parameter corresponding to $\hat{u}_0$ in the φ^4 lattice model whose effect can be studied as a function of $\hat{u}_0$. Therefore it is difficult or even impossible to interpret these solutions in the sense of the scaling structure (119). The solution of reference [5] was only discussed in terms of the usual scaling form (79). This led to the conclusion that usual finite-size scaling in the sense of (79) does not hold for $d > 4$.

In reference [6] the solution for $d > 4$ was first discussed in terms of a single scaling variable tL^2 which led to Figure 7 with a non-scaling plot for $d = 5$. Then an attempt was made to account for the effect of a dangerous irrelevant variable by *afterwards* introducing a variable parameter u into the solution. This parameter corresponds to our $\hat{u}_0 n$. The resulting susceptibility χ_{SR} of Shapiro and Rudnick [6] for this modified version of the spherical model for $d > 4$ reads (see their Eqs. (114, 60))

$$\chi_{SR} = L^2 \left\{ f\left(L^2\tilde{t},\ uL^{4-d}\right)\right\}^{-1}, \quad (149)$$

$$\tilde{t} = t - \tilde{K}L^{2-d}, \quad (150)$$

where the amplitude

$$\tilde{K} = T_c\left[A_1 - 2(d-2)^{-1}(2\pi J)^{-1}\right] \quad (151)$$

is a constant (see also Eqs. (47, 10) of Ref. [7]). The structure of the t and L dependence of χ_{SR} disagrees with that of our $\hat{\chi}$. A disagreement exists also with regard to the dependence on the coupling u. Our $\delta\hat{r}$ (corresponding to $\tilde{t}$) contains the coupling $\hat{u}_0 n$ in the second term on the r.h.s. of (136), *i.e.*, $L^2\delta\hat{r} = F(L^2 t, \hat{u}_0 n L^{4-d})$ whereas $\tilde{K}$ in (151) is *independent of* u. Thus, $L^2\tilde{t} = \Phi(L^2 t, \tilde{K}L^{4-d}) \neq \Psi(L^2 t, uL^{4-d})$. The crucial consequence is that the structure of (149, 150) is incorrect since it does not have the general finite-size scaling form (119) whose validity we have proven for the φ^4 lattice model for $d > 4$. We recall that the u dependence that should enter $\tilde{K}$ does *not* have a dangerous irrelevant character since it originates from the $\mathbf{k} \neq \mathbf{0}$ modes, as demonstrated by our exact solution $\hat{\chi}$ in (91) where $\hat{\Delta}$, equation (94), in the form of equation (96) corresponds to the term $\tilde{K}L^{2-d}$ in (150). A clear distinction between $\mathbf{k} = \mathbf{0}$ and $\mathbf{k} \neq \mathbf{0}$ modes has not been made in the procedure of introducing u in Appendix B of reference [6] which failed to introduce a u-dependence into the amplitude $\tilde{K}$.

Finally we comment on the claim [6] that for $d > 4$ the finite spherical model and the lowest-mode approach ("rounded mean field theory" [6]) yield identical predictions near T_c. This statement is incorrect for the region $\hat{a}_0 t L^2 > 0$ (compare our Eqs. (102, 104)).

7 Discussion

We have studied the field-theoretic version and the lattice version of the $O(n)$ symmetric φ^4 model in the large-n limit for a d-dimensional hypercubic geometry with periodic boundary conditions. Essential parts of our conclusions will apply also to other geometries and will have an important impact also on the case of a finite number of components of the order parameter. Explicit results of this kind have been presented recently [13] for $n = 1$ which can be extended to $n > 1$ on the basis of reference [26]. Further results are derived in reference [25]. We discuss the following five aspects of our conclusions.

(i) We have shown on the basis of an analysis of leading finite-size effects on the susceptibility, the order parameter and the specific heat that lattice effects are important above the upper critical dimension. The effect of the lattice manifests itself not only in a change of nonuniversal amplitudes (as expected) but also in a change of the exponents of the leading finite-size terms as compared to the exponents of the field-theoretic description. This unexpected feature has not been noticed previously in the literature and is of importance from the point of view of both statistical physics and continuum field theory.

(ii) Our results confirm that finite-size scaling in its usual simple form does not hold for $d > 4$, as expected [5], and that instead a generalized finite-size scaling form is valid with two reference lengths. As an unexpected result we have found that the corresponding finite-size scaling functions of the field-theoretic model are nonuniversal. In particular, the scaling functions of the φ^4 field theory and of the φ^4 lattice model differ significantly in structure. For the φ^4 lattice Hamiltonian $\hat{H}$, in the large-n limit, the finite-size scaling functions turn out to be independent of the specific form of the lattice interaction; the latter enters only the amplitude of the correlation length $\hat{\xi}_0$, equation (142), and the reference length $\hat{l}_0$, equation (141). It remains to be seen whether this kind of restricted universality holds also for finite n [25]. Further studies with different forms of $\hat{H}$ are needed to determine the class of lattice models for which universal finite-size scaling functions (in a restricted sense) exist above the upper critical dimension.

(iii) Although previous arguments in support of the asymptotic correctness of the lowest-mode approach for $d > 4$ [17] have been widely accepted in the literature on finite-size effects in statics [3,6,7,10,12,18,19,27–34] and dynamics [19,35–39] we have shown that these arguments are not generally valid. The lowest-mode approach takes into account only homogeneous fluctuations [17] and predicts incorrect exponents for the leading finite-size effects on the susceptibility, order-parameter and specific heat of the field-theoretic model for $d > 4$. For the lattice model, it fails for the leading finite-size terms of the susceptibility and order parameter above T_c, and of the specific heat at T_c. Thus the inhomogeneous fluctuations play a more important role above the upper critical dimension than anticipated previously.

(iv) Our results have an impact on the interpretation of Monte-Carlo simulations of spin models on finite lattices above the upper critical dimension [18,30–33] We have shown [13] that a description of these lattice systems in terms of the field-theoretic Hamiltonian H, equation (1), is not correct as far as finite-size effects are concerned, and that instead a lattice Hamiltonian $\hat{H}$ should be employed. It remains to be seen whether the previous asymptotic values of certain ratios [17] can be justified on the basis of a lattice Hamiltonian. In any case there remains the problem of predicting the form of the non-asymptotic (finite L) corrections. Previous analyses [18,30–33] that are based on the field-theoretic Hamiltonian H are not conclusive in this respect. Detailed knowledge of the structure of these corrections including the predictability of their amplitudes is of importance for the analysis of finite-size data of Monte-Carlo simulations. It is not established whether the form of the lattice Hamiltonian in (34) for $n = 1$ is appropriate and sufficient to explain the leading non-asymptotic correction terms, *e.g.*, of the Binder cumulant of the five-dimensional Ising model.

(v) Although we have not yet discussed the more complicated border-line case $d = d_u$ we expect on the basis of our present results that lattice effects on the leading finite-size terms are non-negligible also for $d = d_u$ in that they will affect the amplitudes in a nontrivial way (different from the cases $d < d_u$ and $d > d_u$). This may yield testable theoretical predictions and may be of particular relevance near tricritical points whose border-line dimension is $d_u = 3$. There may also be relevant applications at $d_u = 4$ in models of elementary particle physics.

Finally we mention that it would be interesting to examine the crossover from the critical finite-size regime to the regime of finite-size rounding near the coexistence line below T_c where Goldstone modes govern the long-distance properties [5,7,17,26].

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Appendix: Large L behavior of $\varDelta$

The quantity $\varDelta$, equation (90), can be written as

$$\varDelta = 4u_0 n \varLambda^{d-2} \varDelta_0 \tag{A.1}$$

where

$$\varDelta_0(\varLambda L) = \varLambda^{2-d}\Big[\int_{\mathbf{k}} \mathbf{k}^{-2} - L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}} \mathbf{k}^{-2}\Big] \tag{A.2}$$

is a dimensionless function that depends only on $\varLambda L$ and d. Using the dimensionless vektor $\mathbf{k}/\varLambda$ and the representation

$$(\mathbf{k}/\varLambda)^{-2} = \int_0^\infty dx\, e^{-(\mathbf{k}/\varLambda)^2 x} = \int_0^\infty dx \prod_{j=1}^{d} \Big[e^{-(k_j/\varLambda)^2 x}\Big] \tag{A.3}$$

we obtain

$$\varDelta_0 = \int_0^\infty dx \Big[S(\infty,x)^d - S(\varLambda L,x)^d + (\varLambda L)^{-d}\Big] \tag{A.4}$$

with

$$S(\varLambda L, x) = (\varLambda L)^{-1} \sum_q \exp(-q^2 x) \tag{A.5}$$

where the (one-dimensional) sum $\sum_q$ runs over $q = 2\pi m/(\varLambda L)$ with $m = 0, \pm1, \pm2,$ ... in the range $-1 \le q < 1$. For $\varLambda L \to \infty$ we have

$$S(\infty, x) = \frac{1}{2\pi}\int_{-1}^{1} dq \exp(-q^2 x). \tag{A.6}$$

In determining the large $\varLambda L$ behavior of $\varDelta_0$ it is important to distinguish the regimes $0 \le x \lesssim \varLambda L$ and $x \gtrsim \varLambda L$ in the integral representation of (A.4). Accordingly we split

$$\varDelta_0 = \varDelta_1 + \varDelta_2 \tag{A.7}$$

where

$$\varDelta_1 = \int_0^{\varLambda L} dx \big[S(\infty,x)^d - S(\varLambda L,x)^d + (\varLambda L)^{-d}\big], \tag{A.8}$$

$$\varDelta_2 = \int_{\varLambda L}^{\infty} dx \big[S(\infty,x)^d - S(\varLambda L,x)^d + (\varLambda L)^{-d}\big]. \tag{A.9}$$

First we derive the leading ΛL dependence of Δ_2. By a simple change of variables we rewrite Δ_2 as

$$\Delta_2 = \frac{(\Lambda L)^{2-d}}{4\pi^2} \int_{y_0}^{\infty} dy \Big\{ \Big[\widetilde{S}(y, \Lambda L\sqrt{y})\Big]^d - \Big[\sum_m e^{-ym^2}\Big]^d + 1 \Big\} \tag{A.10}$$

with $y_0 = 4\pi^2/(\Lambda L)$ and

$$\widetilde{S}(y,z) = \frac{2}{\sqrt{y}} \int_0^{z/(2\pi)} \exp(-t^2)dt. \tag{A.11}$$

The sum $\sum_m$ in (A.10) runs over $m = 0, \pm1, \pm2, \ldots$ in the range $-\Lambda L/(2\pi) \leq m < \Lambda L/(2\pi)$. For $y \gg y_0/(\Lambda L)$ this sum can be transformed as

$$\sum_m e^{-ym^2} = K(y) + \mathcal{O}(e^{-\Lambda L y/y_0}) \tag{A.12}$$

with

$$K(y) = \sum_{m=-\infty}^{\infty} \exp(-ym^2). \tag{A.13}$$

For $y \gg y_0/(\Lambda L)$ we can also simplify

$$\widetilde{S}(y, \Lambda L\sqrt{y}) = (\pi/y)^{1/2} + \mathcal{O}(y^{-1/2}\, e^{-\Lambda L y/y_0}). \tag{A.14}$$

This leads to

$$\Delta_2 = \frac{(\Lambda L)^{2-d}}{4\pi^2} \int_{y_0}^{\infty} dy \Big\{ \Big(\frac{\pi}{y}\Big)^{d/2} - [K(y)]^d + 1 + \mathcal{O}\left(y^{-1/2} e^{\Lambda L y/y_0}\right)\Big\}. \tag{A.15}$$

From Poisson's summation formula we have [17]

$$K(y) = (\pi/y)^{1/2}\, K(\pi^2/y) \tag{A.16}$$
$$= (\pi/y)^{1/2}\left[1 + \mathcal{O}\left(e^{-\pi^2/y}\right)\right], \tag{A.17}$$

thus at $y = y_0$ the integrand of (A.15) is

$$1 + \mathcal{O}(y_0^{-1/2}\, e^{-\pi^2/y_0}) + \mathcal{O}(y_0^{-1/2}\, e^{-\Lambda L}) \tag{A.18}$$

where the last two contributions remain negligible in the limit $y_0 \to 0$ corresponding to $\Lambda L \to \infty$. This leads to the large ΛL behavior

$$\Delta_2 = (\Lambda L)^{2-d}\left[a_2(d) + \mathcal{O}(e^{-\Lambda L})\right] - (\Lambda L)^{1-d} \tag{A.19}$$

with

$$a_2(d) = \frac{-1}{4\pi^2} \int_0^{\infty} dy \big[K(y)^d - (\pi/y)^{d/2} - 1\big]. \tag{A.20}$$

In order to determine the leading ΛL dependence of Δ_1 we first derive a representation of the one-dimensional integral

$$I(a,b) = \int_a^b f(x)dx \tag{A.21}$$

in terms of summations. We assume the arbitrary real function $f(x)$ of the real variable x to be well behaved in the interval $a \leq x \leq b$, in particular we assume that $f(x)$ has a convergent Taylor expansion around any x in this interval. We split the interval $a \leq x \leq b$ into N subintervals of length $\Delta x = (b-a)/N$ between the points $x_i = a + i\Delta x$, $i = 0, 1, \ldots, N$, with $x_0 = a, x_N = b$. The integral I can be represented as

$$I(a,b) = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x)dx. \tag{A.22}$$

For each interval we expand $f(x)$ into a Taylor series

$$\int_{x_i}^{x_{i+1}} f(x)dx = \int_{x_i}^{x_{i+1}} \left[f(x_i) + \sum_{n=1}^{\infty} \frac{1}{n!} f^{(n)}(x_i)(x-x_i)^n\right] dx \tag{A.23}$$

$$= f(x_i)\Delta x + \sum_{n=1}^{\infty} \frac{1}{(n+1)!} f^{(n)}(x_i)(\Delta x)^{n+1} \tag{A.24}$$

where $f^{(n)}(x) \equiv d^n f(x)/dx^n$. Thus we obtain

$$\int_a^b f(x)dx = \sum_{i=0}^{N-1} f(x_i)\Delta x + \sum_{n=1}^{\infty} \frac{(\Delta x)^n}{(n+1)!} I_N^{(n)}(a,b) \tag{A.25}$$

where

$$I_N^{(n)}(a,b) = \sum_{i=0}^{N-1} f^{(n)}(x_i)\Delta x. \tag{A.26}$$

Since $f(x)$ is an arbitrary function we may also apply (A.25) to the function $f'(x)$ instead of $f(x)$. This yields an expression for $I_N^{(1)}(a,b)$ in terms of higher derivatives,

$$I_N^{(1)}(a,b) = f(b) - f(a) - \sum_{n=1}^{\infty} \frac{(\Delta x)^n}{(n+1)!} I_N^{(n+1)}(a,b), \tag{A.27}$$

which can be substituted into the $n = 1$ term of (A.25). Successive application of this procedure permits one to express the difference

$$\int_a^b f(x)dx - \sum_{i=0}^{N-1} f(x_i)\Delta x \equiv R_N(a,b) \tag{A.28}$$

in terms of the differences of the derivatives at a and b,

$$\Delta f^{(k)} = f^{(k)}(b) - f^{(k)}(a). \tag{A.29}$$

The result is

$$R_N(a,b) = \frac{\Delta x}{2}\left[f(b) - f(a)\right] - \frac{(\Delta x)^2}{12}\Delta f^{(1)} + \frac{(\Delta x)^4}{720}\Delta f^{(3)} + \mathcal{O}\left((\Delta x)^6\right). \tag{A.30}$$

The coefficients of the $\mathcal{O}\left((\Delta x)^3\right)$ and $\mathcal{O}\left((\Delta x)^5\right)$ terms vanish. Since $\Delta x \sim \mathcal{O}(N^{-1})$ this representation is expected to converge rapidly for large N if $\Delta f^{(k)}$ remains sufficiently well-behaved for large k.

We apply (A.28–A.30) to the integral $S(\infty, x)$ in (A.6) where the integration variables q plays the role of x in (A.21–A.30). The sum corresponding to (A.26) is $S(\Lambda L, x)$, equation (A.5), with $2\pi/(\Lambda L)$ corresponding to Δx. We obtain

$$S(\infty, x) = S(\Lambda L, x) + \frac{2\pi}{3} x e^{-x}(\Lambda L)^{-2} + (2\pi)^3\left(\frac{1}{30}x^2 - \frac{1}{45}x^3\right) e^{-x}(\Lambda L)^{-4} + \mathcal{O}\left((\Lambda L)^{-6}\right). \tag{A.31}$$

Substitution into (A.8) and evaluating the integral over x for large ΛL yields the leading terms

$$\Delta_1 = a_1(d)(\Lambda L)^{-2} + (\Lambda L)^{1-d} + \mathcal{O}\left((\Lambda L)^{-4},\, e^{-\Lambda L}\right) \tag{A.32}$$

where

$$a_1(d) = \frac{d}{3(2\pi)^{d-2}} \int_0^\infty dx\, x e^{-x}\left[\int_{-1}^{1} dy\, e^{-y^2 x}\right]^{d-1}. \tag{A.33}$$

Together with (A.19) for Δ_2 this leads to (95) for Δ .

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