

ELECTRONIC PROPERTIES OF SOLID

Finite-Size Scaling from the Self-Consistent Theory of Localization¹

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Abstract—Accepting the validity of Vollhardt and Wölfle’s self-consistent theory of localization, we derive the finite-size scaling procedure used for studying the critical behavior in the d -dimensional case and based on the consideration of auxiliary quasi-1D systems. The obtained scaling functions for $d = 2$ and $d = 3$ are in good agreement with numerical results: it signifies the absence of substantial contradictions with the Vollhardt and Wölfle theory on the level of raw data. The results $\nu = 1.3–1.6$, usually obtained at $d = 3$ for the critical exponent of the correlation length, are explained by the fact that dependence $L + L_0$ with $L_0 > 0$ (L is the transversal size of the system) is interpreted as $L^{1/\nu}$ with $\nu > 1$. The modified scaling relations are derived for dimensions $d \geq 4$; this demonstrates the incorrectness of the conventional treatment of data for $d = 4$ and $d = 5$, but establishes the constructive procedure for such a treatment. The consequences for other finite-size scaling variants are discussed.

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1. INTRODUCTION

The contemporary situation in investigating Anderson localization is characterized by the fact that the results of numerical modeling (see [1]) contradict all other information on the critical behavior [1–3]. Such situation is unacceptable, since it undermines the belief in analytical theory.

The critical behavior of conductivity σ and the correlation length ξ

$$\sigma \propto \tau^s, \quad \xi \propto |\tau|^{-\nu} \quad (1)$$

(τ is the distance to the transition point) obtained from Vollhardt and Wölfle’s self-consistent theory of localization by [4, 5], has the form

$$\nu = \begin{cases} 1/(d-2), & 2 < d < 4 \\ 1/2, & d > 4 \\ s = 1, & 2 < d < \infty \end{cases} \quad (2)$$

(d is the dimension of space), and in fact summarizes all known results. Indeed, formula (2)

(a) distinguishes values $d_{c1} = 2$ and $d_{c2} = 4$ as the lower and upper critical dimensions, which are known from independent arguments (see [2, 6] for details);

(b) agrees with the theory for $d = 2 + \epsilon$ [7],

$$\nu = \frac{1}{\epsilon} - 0 \cdot \epsilon^0 + 0 \cdot \epsilon^1 + O(\epsilon^2); \quad (3)$$

(c) satisfies the Wegner scaling relation $s = (d-2)\nu$ [8] for $d < d_{c2}$;

(d) gives independent of d critical exponents for $d > d_{c2}$, as is typical for mean-field theory;

(e) agrees with the results $\nu = 1/2$ [9, 10] and $s = 1$ [11] for $d = \infty$;

(f) agrees with the experimental results $s \approx 1$, $\nu \approx 1$ for $d = 3$, obtained by measuring the conductivity and dielectric susceptibility [12, 13].²

It is clear that the Vollhardt and Wölfle theory gives at least a very successful approximation that satisfies all general principles and reproduces all known results. Moreover, the suspicion arises that result (2) is exact [14].³ This conjecture is supported by [16], where Eq. (2) is derived without model approximations on the basis of symmetry analysis.

As for numerical results [17–31], they can be summarized by the empirical formula $\nu \approx 0.8/(d-2) + 0.5$ [25], which has evident fundamental defects. Recent developments make the situation even worse, giving for $d = 3$ values of $\nu = 1.54 \pm 0.08$ [24], $\nu = 1.45 \pm 0.08$ [26], $\nu = 1.40 \pm 0.15$ [27], $\nu = 1.57 \pm 0.02$ [29], etc.

In our opinion, this means the existence of serious defects in conventional numerical algorithms. It is not reasonable to question the raw data that have been obtained independently by many groups; however, it is possible to doubt the algorithms themselves, which are not based on any serious theory. In particular, there is

² Paper [13] is especially interesting, since the experiment has been performed for nondegenerate electron gas and the influence of interaction can be controlled explicitly.

³ According to Wegner [15], the term ϵ^2 in (3) is finite and large negative. However, this result was derived for the zero-component σ -model, whose correspondence with the initial disordered system is approximate and valid for small ϵ ; so a difference can arise in a certain order in ϵ .

¹ The article was translated by the author.

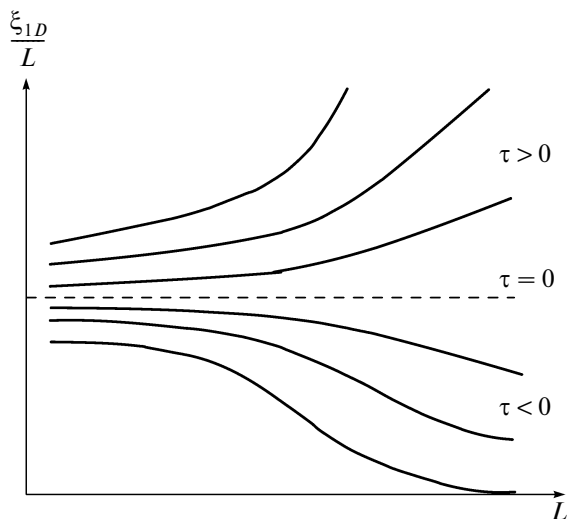


Fig. 1. Dependence of scaling parameter ξ_{1D}/L on transversal size L of the system.

a possibility of rough violation of scaling [32] or the existence of a large characteristic length scale [3, 33].

In the present paper, the following approach is accepted. We suppose that the Vollhardt and Wölfle theory (Section 2) is correct (there are real grounds for such an assumption [16]) and derive the quantities that are immediately “measured” in numerical experiments. Then comparison can be made on the level of the raw data, avoiding the suspicious treatment procedure.

We restrict the discussion to the popular variant of finite-size scaling based on consideration of auxiliary quasi-1D systems [34]. Thus, instead of the infinite 3D system, we consider the system of size $L \times L \times L_z$, where $L_z \rightarrow \infty$. Such a system is topologically one-dimensional and does not possess long-range order, so the corresponding correlation length ξ_{1D} is finite. If ξ_{1D} can be calculated, then its dependence at $L \rightarrow \infty$ makes it possible to reveal phase transitions in the initial 3D system: it appears that $\xi_{1D}/L \rightarrow \infty$ in the phase with long-range order and $\xi_{1D}/L \rightarrow 0$ in the phase with short-range correlations [32, 34]. In the numerical studies, the following scaling relation is usually postulated

$$\frac{\xi_{1D}}{L} = F\left(\frac{L}{\xi}\right). \quad (4)$$

It is based on the assumption that the correlation length ξ of the considered d -dimensional system is the only essential length scale, so L enters only in the combination L/ξ . If this relation is valid, then the quantity ξ_{1D}/L depends on L in accordance with Fig. 1: it remains constant at the critical point, while all curves for $\tau > 0$ (and correspondingly $\tau < 0$), it can be reduced to one universal curve by scale transformation. If two curves for $\tau = \tau_1$ and $\tau = \tau_2$ are calculated,

then the scale transformation makes it possible to determine the ratio of two correlation lengths. Taking succession $\tau_0, \tau_1, \tau_2, \dots$, we can determine $\xi(\tau)$ apart from the numerical factor and investigate its critical behavior.

We demonstrate below that scaling relation (4) is indeed valid in the limit of large ξ and L for space dimensions $d < 4$, while calculation of the scaling function F for $d = 2$ and $d = 3$ shows a good agreement with numerical results (Section 3). It signifies that the Vollhardt and Wölfle theory is confirmed on the level of raw data. Section 4 clarifies why values of the exponent ν in the numerical experiments for $d = 3$ are always greater than unity: in the vicinity of the critical point the scaling parameter ξ_{1D}/L behaves as $\tau(L + L_0)$ with $L_0 > 0$, which is conventionally interpreted as $\tau L^{1/\nu}$ with $\nu > 1$.

For higher dimensions, the scaling relation (4) cannot be correct, and it can be stated on the level of a theorem. The problem of the Anderson transition can be exactly reduced to the ϕ^4 field theory [6, 35–37], which is non-renormalizable for $d > 4$ [38, 39]. Therefore, the ultraviolet cut-off (i. e. atomic scale) cannot be excluded from results, and ξ is certainly not the only relevant length scale. However, it is possible to derive the modified scaling relations

$$y = F(x) \quad (5)$$

with

$$y = \frac{\xi_{1D}}{L} \left(\frac{a}{L}\right)^{(d-4)/3}, \quad (6)$$

$$x = \frac{\xi}{L} \left(\frac{a}{L}\right)^{(d-4)/3}, \quad d > 4$$

and

$$y = \frac{\xi_{1D}}{L} \left[\ln\left(\frac{L}{a}\right)\right]^{-1/3}, \quad (7)$$

$$x = \frac{\xi}{L} \frac{[\ln(L/a)]^{1/6}}{[\ln(\xi/a)]^{1/2}}, \quad d = 4,$$

demonstrating the incorrectness of conventional data treatment for $d = 4$ and $d = 5$ [1], but establishing the constructive procedure for such treatment (Section 5). Modified scaling (5) with

$$y = \frac{\xi_{1D}}{L} \left[\frac{\epsilon}{1 - (L/a)^{-\epsilon}} \right]^{1/3}, \quad (8)$$

$$x = \frac{\xi}{L} \frac{[1 - (L/a)^{-\epsilon}]^{1/6} \epsilon^{1/3}}{[(\xi/a)^{\epsilon} - 1]^{1/2} (L/a)^{-\epsilon/2}}, \quad d = 4 - \epsilon,$$

can also be derived for $d = 4 - \epsilon$ dimensions. It can be used for alternative treatment at $d = 3$, in order to estimate the systematic errors related to the possible existence of the large length scale. Finally, in Section 6 we discuss some consequences of the present analysis for other variants of finite-size scaling.

2. VOLLHARDT AND WÖLFLE THEORY

The Vollhardt and Wölfle theory is based on the existence of the diffusion pole in the irreducible four-leg vertex $U_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$,

$$U_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = U_{\mathbf{k}\mathbf{k}'}^{\text{reg}}(\mathbf{q}) + \frac{F(\mathbf{k}, \mathbf{k}', \mathbf{q})}{-i\omega + D(\omega, \mathbf{k} + \mathbf{k}')(\mathbf{k} + \mathbf{k}')^2}, \quad (9)$$

entering the Bethe–Salpiter equation and playing the role of the scattering probability $W_{\mathbf{k}\mathbf{k}'}$ in the quantum kinetic equation. Neglecting the spatial dispersion of the diffusion coefficient⁴ and using the estimate in the spirit of the τ -approximation, $D \propto \langle U \rangle^{-1}$, where $\langle \dots \rangle$ is averaging over momenta, we arrive at the self-consistency equation of the Vollhardt and Wölfle theory

$$D \sim \left[U_0 + F_0 \int \frac{d^d q}{-i\omega + D(\omega, q)q^2} \right]^{-1}. \quad (10)$$

It can be obtained by approximate solution of the Bethe–Salpiter equation [4], or by accurate analysis of the spectral properties of the quantum collision operator [16]. It can be written in a physically clear form if the coefficients are estimated for weak disorder (which is actual for lower dimensions) and the following situation near the band center in the Anderson model is implied:

$$\frac{E^2}{W^2} = \frac{D}{D_{\min}} + \Lambda^{2-d} \int_{|q| < \Lambda} \frac{d^d q}{(2\pi)^d} \frac{1}{(-i\omega/D) + q^2}. \quad (11)$$

Here E is the energy of the bandwidth order, W is the amplitude of disorder, Λ is the ultraviolet cutoff, and D_{\min} is the characteristic scale of the diffusion coefficient corresponding to minimal Mott conductivity. Generally, some monotonic function of W appears in the left-hand side, but it is not essential for subsequent considerations.

Let us introduce the basic integral

$$I(m) = \int_{|q| < \Lambda} \frac{d^d q}{(2\pi)^d} \frac{1}{m^2 + q^2}, \quad (12)$$

which can be estimated for $m \ll \Lambda$ as

$$I(m) = \begin{cases} c_d/m^{2-d}, & d < 2 \\ c_2 \ln(\Lambda/m), & d = 2 \\ I(0) - c_d m^{d-2}, & 2 < d < 4 \\ I(0) - c_4 m^2 \ln(\Lambda/m), & d = 4 \\ I(0) - c_d m^2 \Lambda^{d-4}, & d > 4, \end{cases} \quad (13)$$

⁴ Such a possibility was justified in [16]. Attempts to relate the spatial dispersion of the diffusion coefficient with the multifractality of wavefunctions [41] ignore the complex-valuedness of the diffusion coefficient and its complicated rearrangement near transition [42].

where

$$c_d = \begin{cases} \pi K_d / (2 \sin(\pi d/2)), & d < 2 \\ 1/2\pi, & d = 2 \\ \pi K_d / |2 \sin(\pi d/2)|, & 2 < d < 4 \\ 1/(8\pi^2), & d = 4 \\ K_d / (d-4), & d > 4 \end{cases} \quad (14)$$

and $K_d = [2^{d-1} \pi^{d/2} \Gamma(d/2)]^{-1}$ is the surface of the d -dimensional unit sphere divided by $(2\pi)^d$. The metallic phase is possible when the value of $I(0)$ is finite, i.e., for $d > 2$. Accepting $D = \text{const} > 0$ for $\omega \rightarrow 0$ and specifying τ as a distance to transition, we have

$$D = D_{\min} \tau, \quad \tau = \frac{E^2}{W^2} - I(0) \Lambda^{2-d}; \quad (15)$$

i.e., the exponent of conductivity is unity, in agreement with formula (2). In the dielectric phase we perform the substitution

$$D = -i\omega \xi^2, \quad \xi = m^{-1}, \quad (16)$$

where ξ is the correlation length. Then Eq. (11) gives

$$\begin{aligned} \xi &\sim a \frac{E^2}{W^2}, & d = 1, \\ \xi &\sim a \exp\left(2\pi \frac{E^2}{W^2}\right), & d = 2, \\ \xi &\sim a |\tau|^{-\nu}, & d > 2, \end{aligned} \quad (17)$$

with the exponent ν defined by Eq. (2). In what follows, we accept $a = \Lambda^{-1}$, so that a is the atomic length scale, not necessarily coinciding with the lattice spacing.

3. SCALING FUNCTIONS FOR $d < 4$

3.1. Definition of Scaling Functions

For description of quasi-1D systems, it is sufficient to represent the basic integral (12) in the following form:

$$I(m) = \frac{1}{L^{d-1}} \sum_{|q_{\perp}| < \Lambda_{\perp}} \int_{|q_{\parallel}| < \Lambda_{\parallel}} \frac{dq_{\parallel}}{2\pi} \frac{1}{m^2 + q_{\parallel}^2 + q_{\perp}^2}, \quad (18)$$

$$m^{-1} = \xi_{1D},$$

where d -dimensional vector $q = (q_1, q_2, \dots, q_d)$ is replaced by its transversal and longitudinal components

$$q_{\perp} = (q_1, q_2, \dots, q_{d-1}), \quad q_{\parallel} = q_d, \quad (19)$$

and the former is considered discrete, running the usual allowed values. The term with $q_{\perp} = 0$ has divergence m^{-1} for $m \rightarrow 0$, so that the system is always localized.

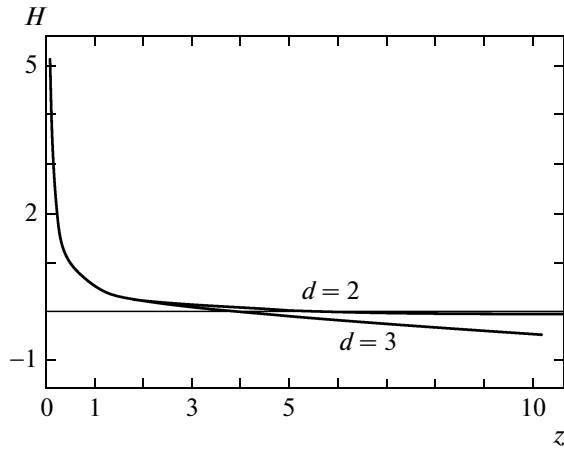


Fig. 2. Function $H(z)$ for $b_1 = 0$ in two and three dimensions.

After integration over q_{\parallel} , the following decomposition is convenient:

$$\begin{aligned}
 I(m) &= \frac{1}{L^{d-1}} \frac{1}{\pi m} \arctan \frac{\Lambda}{m} + \frac{1}{\pi L^{d-1}} \\
 &\times \sum_{\substack{q_{\perp} \neq 0 \\ |q_{\perp}| < \Lambda}} \left(\frac{1}{\sqrt{m^2 + q_{\perp}^2}} \arctan \frac{\Lambda}{\sqrt{m^2 + q_{\perp}^2}} \right. \\
 &\left. - \frac{1}{|q_{\perp}|} \arctan \frac{\Lambda}{|q_{\perp}|} \right) + \frac{1}{\pi L^{d-1}} \sum_{\substack{q_{\perp} \neq 0 \\ |q_{\perp}| < \Lambda}} \frac{1}{|q_{\perp}|} \\
 &\times \arctan \frac{\Lambda}{|q_{\perp}|} \equiv I_1(m) + I_2(m) + I_3(0).
 \end{aligned} \quad (20)$$

We separate the term with $q_{\perp} = 0$, while the remaining sum is rearranged by subtraction and addition of the analogous sum with $m = 0$. In the first term, we trivially have

$$I_1(m) = \frac{1}{L^{d-2}} \left\{ \frac{1}{2mL} + O\left(\frac{a}{L}\right) \right\}. \quad (20')$$

The second term can be transformed by taking the limit $\Lambda \rightarrow \infty$ and substituting $q_{\perp} = 2\pi\mathbf{s}/L$, where $\mathbf{s} = (s_1, \dots, s_{d-1})$ is a vector with integer components $s_i = 0, \pm 1, \pm 2, \dots$:

$$\begin{aligned}
 I_2(m) &= \frac{1}{L^{d-2}} H_0(mL) + O(m^2 \Lambda^{d-4}), \\
 H_0(z) &= \frac{1}{4\pi} \sum_{\mathbf{s} \neq 0} \left(\frac{1}{\sqrt{|\mathbf{s}|^2 + (z/2\pi)^2}} - \frac{1}{|\mathbf{s}|} \right).
 \end{aligned} \quad (21)$$

The third term can be estimated at $L \rightarrow \infty$ by replacing the summation by integration. For finite L and $d > 2$, it has the structure

$$I_3(0) = \Lambda^{d-2} \left\{ b_0 + b_1 \left(\frac{a}{L}\right)^{d-2} + b_2 \left(\frac{a}{L}\right)^{d-1} + \dots \right\}. \quad (22)$$

Substituting formulas (20)–(22) in the self-consistency equation (11), we have for $d > 2$

$$\begin{aligned}
 \left(\frac{L}{a}\right)^{d-2} [\tau + O(m^2 a^2)] + O\left(\frac{a}{L}\right) \\
 = b_1 + H_0(mL) + \frac{1}{2mL},
 \end{aligned} \quad (23)$$

where we replace

$$\tau = \frac{E^2}{W^2} - b_0, \quad (24)$$

in agreement with definition (15), since b_0 corresponds to $I(0)$, calculated in the integral approximation. Expressing τ through the correlation length ξ of the d -dimensional system ($\xi^{-1/\nu} \sim |\tau| = \pm\tau$) and omitting the terms disappearing at $a \rightarrow 0$, we have

$$\pm c_d \left(\frac{L}{\xi}\right)^{d-2} = H\left(\frac{L}{\xi_{1D}}\right), \quad (25)$$

$$H(z) = b_1 + \frac{1}{4\pi} \sum_{\mathbf{s} \neq 0} \left(\frac{1}{\sqrt{|\mathbf{s}|^2 + (z/2\pi)^2}} - \frac{1}{|\mathbf{s}|} \right) + \frac{1}{2z}, \quad (26)$$

i.e., scaling relation (4) between variables ξ_{1D}/L and ξ/L , consisting of two branches.

For $d = 2$, instead of (22), we have

$$I_3(0) = \frac{1}{2\pi} \ln \frac{L}{a} + b_1 + \dots \quad (22')$$

and, using the result from Section 2,

$$\frac{E^2}{W^2} = \frac{1}{2\pi} \ln \frac{\xi}{a},$$

we obtain the scaling relation in the form

$$\frac{1}{2\pi} \ln \left(\frac{\xi}{L}\right) = H\left(\frac{L}{\xi_{1D}}\right) \quad (27)$$

with the previous definition of $H(z)$. The functions $H(z)$ for $d = 2$ and $d = 3$ are presented in Fig. 2, where $b_1 = 0$ was taken.

3.2. Two-Dimensional Case

For $d = 2$, the constant b_1 can be eliminated by changing the scale for ξ (see below) and we can take $b_1 = 0$. The asymptotics of $H(z)$ for $z \ll 1$ is determined

by the last term in Eq. (26), while for $z \gg 1$, the sum in Eq. (26) can be replaced by the integral

$$H(z) = \begin{cases} \frac{1}{2z}, & z \ll 1 \\ -\frac{1}{2\pi} \ln z + \text{const}, & z \gg 1, \end{cases} \quad (28)$$

so that we have in variables $y = \xi_{1D}/L$ and $x = \xi/L$

$$y = \begin{cases} (1/\pi) \ln x, & x \gg 1 \\ \text{const } x, & x \ll 1. \end{cases} \quad (29)$$

The relation between x and y for their arbitrary values can be found by the numerical calculation of the sum in (26).

The definition of ξ_{1D} and ξ in the Vollhardt and Wölfle theory does not coincide with one used in numerical experiments. In the former case, ξ^2 (and analogously ξ_{1D}^2) is defined as an average $\langle r^2 \rangle$ for the localized eigenfunction $\psi(r)$ [16]. In the latter case, we mean the definition through the asymptotic behavior $\exp\{-r/\xi\}$ of the correlation functions, since ξ_{1D} is calculated as inverse to the minimal Lyapunov exponent⁵; the scale of ξ in numerical experiments is arbitrary from the very beginning. Therefore, in comparing the theory with numerical results, the scales of ξ_{1D} and ξ should be chosen from the best agreement; in log–log coordinates, such fitting reduces to parallel shifts along two axes. The general form of the scaling curve is determined without adjustable parameters.

In Fig. 3, the calculated dependence of ξ_{1D}/L on ξ/L is compared with the pioneer results by MacKinnon and Kramer [18] and the subsequent paper by Schreiber and Ottomeier [19], which is cited as the most detailed investigation of 2D systems in the framework of this algorithm.

3.3. Three-Dimensional Case

The given definition of the sum $I_3(0)$ implies the choice of cut-off in the form of the cylindrical domain ($|q_\perp| < \Lambda$, $|q_\parallel| < \Lambda$). It can be also defined for the spherical ($|q| < \Lambda$) and cubical ($|q_i| < \Lambda$) regions:

$$I_3^{(\text{cub})}(0) = \frac{1}{2\pi^2 L^{d-2}} \sum_{\substack{\mathbf{s} \neq 0 \\ |\mathbf{s}| < \Lambda L/2\pi}} \frac{1}{|\mathbf{s}|} \arctan\left(\frac{\Lambda L}{2\pi|\mathbf{s}|}\right),$$

⁵In general, correspondence between ξ_{1D} and the minimal Lyapunov exponent is not so straightforward [32]; in the present paper, we ignore such complications.

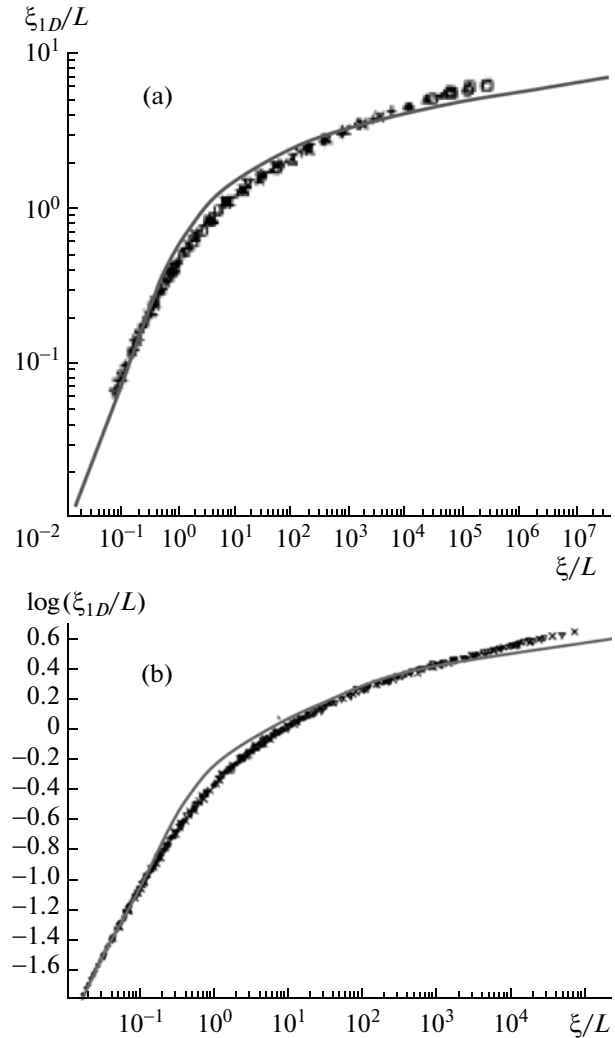


Fig. 3. Comparison of the theoretical scaling curve for $d = 2$ with numerical results by MacKinnon–Kramer [18, Fig. 2a] (a) and Schreiber–Ottomeier [19, Fig. 4] (b).

$$I_3^{(\text{cyl})}(0) = \frac{1}{2\pi^2 L^{d-2}} \times \sum_{\substack{\mathbf{s} \neq 0 \\ |\mathbf{s}| < \Lambda L/2\pi}} \frac{1}{|\mathbf{s}|} \arctan\left(\frac{\Lambda L}{2\pi|\mathbf{s}|}\right), \quad (30)$$

$$I_3^{(\text{sph})}(0) = \frac{1}{2\pi^2 L^{d-2}} \times \sum_{\substack{\mathbf{s} \neq 0 \\ |\mathbf{s}| < \Lambda L/2\pi}} \frac{1}{|\mathbf{s}|} \arctan\left(\frac{\sqrt{(\Lambda L/2\pi)^2 - |\mathbf{s}|^2}}{|\mathbf{s}|}\right).$$

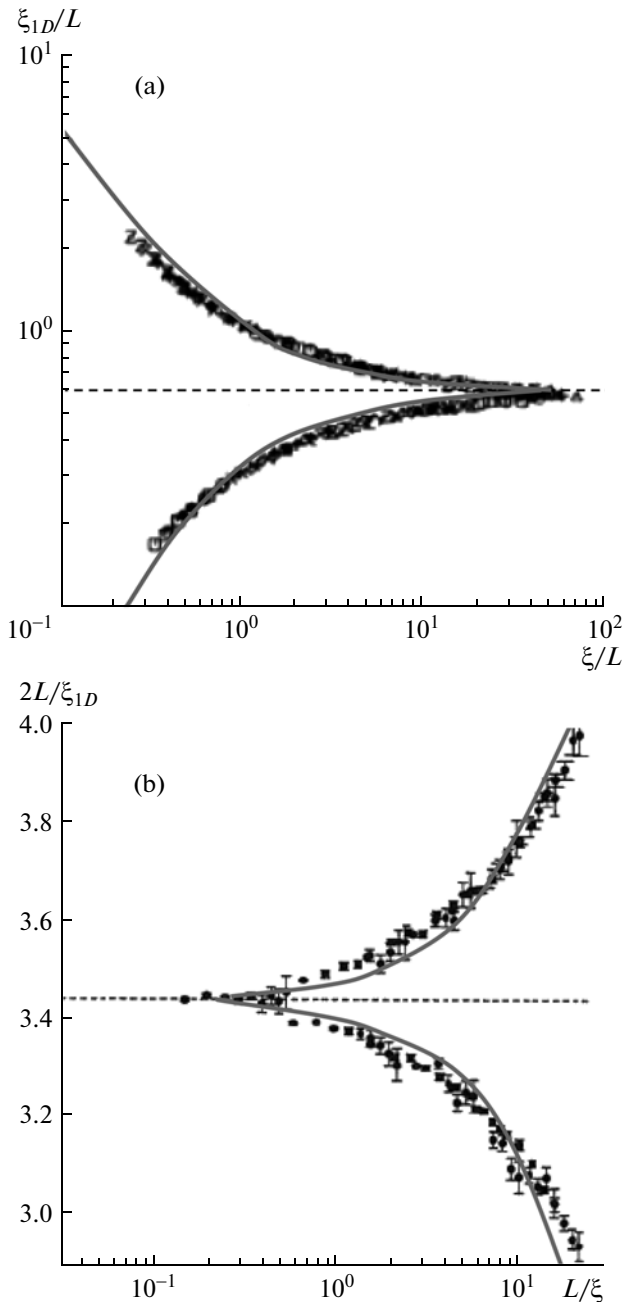


Fig. 4. Comparison of theoretical scaling curves for $d = 3$ with numerical results by MacKinnon–Kramer [18, Fig. 2b] (a) and Markos [1, Fig. 53, right] (b). The values $b_1 = -0.240$ and $b_1 = -0.0718$ were used in the former and the latter case correspondingly.

Numerically we have for these three cases

$$I_3(0) = \begin{cases} 0.0618\Lambda - 0.180L^{-1}, & \text{cube,} \\ 0.0573\Lambda - 0.314L^{-1}, & \text{cylinder,} \\ 0.0507\Lambda - 0.310L^{-1}, & \text{sphere,} \end{cases} \quad (31)$$

i.e., the value of b_1 is not universal but depends on the way of cutoff. The change of this constant allows mak-

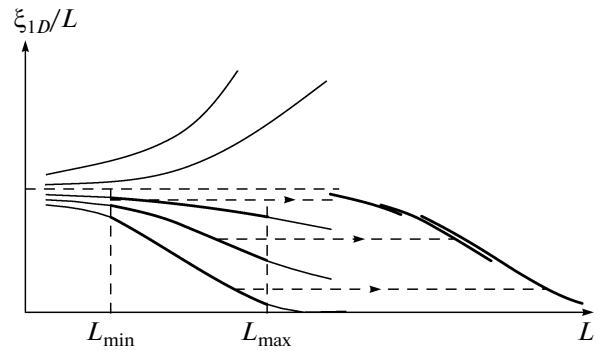


Fig. 5. Construction of scaling curves.

ing the scaling curve more symmetric, or less symmetric; it was chosen from the best agreement,⁶ though its variation in the interval $(-0.3, 0)$ does not significantly affect the results. As in the $2D$ case, the absolute scales for ξ and ξ_{1D} are not fixed by the theory.

Using the asymptotic behavior of $H(z)$

$$H(z) = \begin{cases} 1/2z, & z \ll 1 \\ -A(z - z^*), & z \rightarrow z^* \\ -c_d z^{d-2}, & z \gg 1, \end{cases} \quad (32)$$

we have in variables $y = \xi_{1D}/L$ and $x = \xi/L$

$$y = \begin{cases} 2c_d/x^{d-2}, & y \gg 1 \\ y^* \pm B/x^{d-2}, & y \rightarrow y^* \\ x, & y \ll 1, \end{cases} \quad (33)$$

where z^* and $y^* = 1/z^*$ are the z and y values at the critical point. The same relation, considered in variables y and $1/x$, determines the L dependence of the scaling parameter (Fig. 1), giving two universal curves for $\tau > 0$ and $\tau < 0$, to which all other curves are reduced by the scale transformation:

$$y = \frac{\xi_{1D}}{L} = \begin{cases} \sim \tau L^{d-2}, & y \gg 1 \\ y^* + \text{const } \tau L^{d-2}, & y \rightarrow y^* \\ \xi/L, & y \ll 1. \end{cases} \quad (34)$$

In Fig. 4, the obtained scaling curves are compared with the early results by MacKinnon–Kramer [18] and the more precise results by Markos [1]. In the former case, the agreement is satisfactory; in the latter case, there is a discrepancy on the level of two to three standard deviations. However, we should bear in mind how the scaling curves are constructed: the L dependences for different τ are “measured” in the interval (L_{\min}, L_{\max}) , and then they are fitted to each other by changing the scale (Fig. 5). The full scaling curve is

⁶ The fitting was done by hand (using several reference points) and probably is not optimal.

never present in one experiment, and only separate fragments of it are measured. It is clear from Fig. 4b that the change in scale along the horizontal axis (reduced to a parallel shift in logarithmic coordinates) allows satisfactory fits for the left, right, or middle portion of the curve. It appears that there are no serious contradictions to the Vollhardt and Wölfle theory on the level of raw data.

4. DISCUSSION OF THE SITUATION AT $d = 3$

The interesting question arises: if the Vollhardt and Wölfle theory describes the raw data successfully, then why do all numerical experiments give $\nu > 1$ for $d = 3$?

The history of this question goes back to two papers [17] and [18] by MacKinnon and Kramer, based on the same array of the data. The first of them gives the result

$$\nu = 1.2 \pm 0.3, \quad (35)$$

compatible with the value $\nu = 1$; the second paper confirms this result for a certain fitting procedure, but reports the “more precise” result

$$\nu = 1.50 \pm 0.05, \quad (36)$$

corresponding to the most extremal of present-day values. The first result is based on the analysis of the scaling curve, whose compatibility with the Vollhardt and Wölfle theory is clear from Fig. 4a and has been confirmed by the authors themselves. Further, they indicate that scaling is not satisfactory in the small vicinity of the critical point, and this vicinity was discarded in their treatment. In fact, such a situation is natural, because the small vicinity of the transition is strongly affected by scaling corrections (see Eq. (23)); the latter are small in magnitude but should be compared with the small value of τ . However, the authors of [17, 18] estimated this situation as internally inconsistent and suggested another treatment procedure, which is specially based on analysis of that small region where scaling is absent. Already at this stage it is possible to understand that the latter procedure is unsatisfactory.

Indeed, using systems of restricted L size, we can work straightforwardly only in the regime $\xi \lesssim L$, since in another case, the correlation functions are strongly affected by the finiteness of the system. The use of finite-size scaling allows “jumping over the head” and to advance to the region $\xi \gtrsim L$; however, it is possible only if (a) scaling exists theoretically and (b) it is observed empirically. If either of the two conditions is violated, no such advancement is possible and no experimental information can be obtained on the large ξ region: any manipulations in this region become irrelevant. This conclusion is valid in respect to result (36), since absence of scaling is admitted by the authors. The same conclusion follows from common sense: if value $\nu = 1$ is compatible with the scaling

curve, then it is all the more compatible with the raw data (see the end of Section 3). However, this value is rejected by result (36), and hence the latter should be qualified as essentially incorrect.

The indicated tendencies were continued in other papers. The treatment based on the scaling curves gave rather conservative estimates,⁷ which are not very different from (35). Results close to (36) were stabilized only when the control of scaling was no longer imperative and the analysis of small vicinity of the critical point was generally accepted.

The latter procedure is based on representation of (4) in the form

$$\begin{aligned} \frac{\xi_{1D}}{L} &= F\left(\frac{L^{1/\nu}}{\xi^{1/\nu}}\right) = F(\tau L^{1/\nu}) \\ &\approx y^* + A\tau L^{1/\nu} + \dots; \end{aligned} \quad (37)$$

i.e., the regular expansion in τ is used, motivated by the absence of phase transitions in quasi-1D systems; then the derivative over τ behaves as $L^{1/\nu}$ and gives the exponent ν straightforwardly. Such treatment is correct if the scaling relation (4) is exact. However, it is not exact: linearization of (23) gives

$$\frac{\xi_{1D}}{L} = y^* + A\left(\frac{L}{a}\right)^{d-2} \left[\tau - c \frac{a^2}{\xi_{1D}^2} \right] + O\left(\frac{a}{L}\right). \quad (38)$$

Differentiating over τ and excluding $(\xi_{1D})'_\tau$ from the right-hand side in the iterative manner, we have

$$\left(\frac{\xi_{1D}}{L}\right)'_\tau = A_0 L^{d-2} + A_1 L^{d-6}. \quad (39)$$

Producing subsequent iterations and taking into account further corrections to scaling, we have the following structure of the result:

$$\begin{aligned} \frac{\xi_{1D}}{L} - y^* &= \tau \{ A_0 L^{1/\nu} + A_1 L^{\omega_1} + A_2 L^{\omega_2} + \dots \} \\ &+ B_1 L^{-\gamma_1} + B_2 L^{-\gamma_2} + \dots, \end{aligned} \quad (40)$$

which can be obtained from the general considerations based on the Wilson renormalization group [2].

In three dimensions, the main scaling correction in (39) reduces to a constant and hence

$$\frac{\xi_{1D}}{L} - y^* = A\tau(L + L_0), \quad (41)$$

where the terms disappearing at $L \rightarrow \infty$ are neglected. It is clear from Fig. 6a that Markos' numerical data [1] are excellently fitted by (41). The author himself interpreted them in accordance with (37) and also had good fitting (Fig. 6b).

Such ambiguity of interpretation has a general character. If the combination $A_1 L^{\beta_1} + A_2 L^{\beta_2}$ can be

⁷ As was discussed in [22], the estimate of ν depends on the fragment of the scaling curve used for fitting.

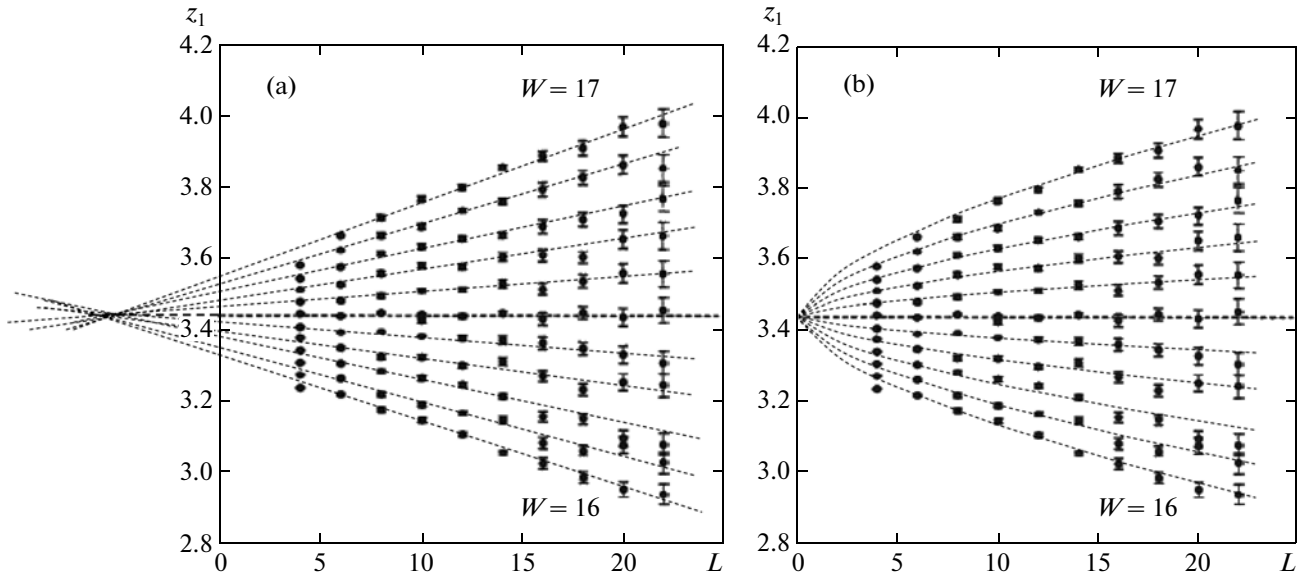


Fig. 6. Numerical data by Markos for $z_1 = 2L/\xi_{1D}$ in the small vicinity of the critical point [1, Fig. 53, left] and their fitting by dependences $(L + L_0)$ (a) and $L^{0.63}$ (b).

linearized in log–log coordinates with the average slope $(\beta_1 + \beta_2)/2$ and the accuracy ϵ , then variation $\beta_1 \rightarrow \beta_1 + \delta$, $\beta_2 \rightarrow \beta_2 - \delta$ preserves the linearity at the same level of accuracy, up to $|\delta| \lesssim |\beta_1 - \beta_2|/2$. If several terms are retained in formulas (40), the situation becomes absolutely uncontrollable: nonlinear fitting with minimization of χ^2 reveals the huge number of minima, and the most in-depth of them is not necessarily correct; a vicinity of any minimum is acceptable if it satisfies the χ^2 criterion. Analysis of all such minima is impossible, and there is no honest procedure to deal with such a situation.⁸ In conclusion, conventional treatment is heavily based on the assumption that only the main term in (40) is essential; the problem of fitting becomes hopeless if additional terms are not negligible.

In the framework of the Vollhardt and Wölfle theory, we have a completely consistent picture. The quantity L_0 violates scaling and empirically has a rather large value, $L_0 \approx 5$ (in lattice units). Good scaling is possible only for $L \gg 5$, and even for the largest systems ($L = 20\text{--}30$), deviations from scaling are described by the parameter $L_0/L \sim 0.2$; so discrepancies in Fig. 4b should be of no surprise. The theoretical value of L_0 is of the order Λ^{-1} with the coefficient depending on the way of cutoff; it is essential that L_0 is positive and limited from below by the atomic scale.

⁸ These questions were discussed [2] in relation to [29]. Nevertheless, this paper continues to be cited [1] as a prominent achievement.

5. SCALING FOR HIGHER DIMENSIONS

5.1. Dimensions $d > 4$

For $d \geq 4$, the sum $I_2(m)$ is divergent at the upper limit and the cutoff parameter Λ cannot be considered infinite. For accurate transformation, we introduce the scale Λ_1 , such as

$$m \ll \Lambda_1 \ll \Lambda, \tag{42}$$

and divide summation in $I_2(m)$ into two regions $|q_\perp| < \Lambda_1$ and $|q_\perp| > \Lambda_1$. In the first region we use the fact that $|q_\perp| \ll \Lambda$, since

$$I_2^{(1)}(m) = -m^2 \frac{1}{2L^{d-1}} \tag{43}$$

$$\times \sum_{\substack{q_\perp \neq 0 \\ |q_\perp| < \Lambda_1}} \frac{1}{|q_\perp| \sqrt{m^2 + q_\perp^2} (|q_\perp| + \sqrt{m^2 + q_\perp^2})}$$

and

$$I_2^{(1)}(m) = \begin{cases} -m^2 \left\{ \frac{K_{d-1} \Lambda_1^{d-4}}{4(d-4)} + O(m^{d-4}) \right\}, & m \gg L^{-1} \\ -m^2 \left\{ \frac{K_{d-1} \Lambda_1^{d-4}}{4(d-4)} + O(L^{4-d}) \right\}, & m \lesssim L^{-1}, \end{cases} \tag{44}$$

i.e., the result is obtained analytically (in the main approximation) for the arbitrary relation between m and L^{-1} . Indeed, for $m \gg L^{-1}$, the sum is estimated by the integral converging at the lower limit already for

$m = 0$; so, finiteness of m gives only small corrections. In the case $m \lesssim L^{-1}$, the main effect from finiteness of L is related to the absence of the term $q_{\perp} = 0$, which can be estimated as restriction $|q_{\perp}| \gtrsim L^{-1}$ in the integral approximation.

In the region $|q_{\perp}| > \Lambda_1$, we make use of condition $|q_{\perp}| \gg m$ and produce expansions in $m/|q_{\perp}|$; after separation of the factor m^2 , we can set $m = 0$ in the sum and estimate it by transformation to the integral

$$I_2^{(2)}(m) = m^2 \frac{K_{d-1} \Lambda_1^{d-4}}{4(d-4)} - cm^2 \Lambda^{d-4}, \quad (44')$$

where c depends on the way of cutoff; dependence on Λ_1 disappears in the sum $I_2^{(1)} + I_2^{(2)}$.

The results for $I_1(m)$ and $I_3(0)$ are the same as in Section 3. The self-consistency equation takes the form

$$\tau \Lambda^{d-2} = \frac{1}{L^{d-2}} \frac{1}{2mL} - cm^2 \Lambda^{d-4}. \quad (45)$$

Substituting $\tau \propto \xi^{-2}$ and introducing variables

$$y = \frac{\xi_{1D}}{L} \left(\frac{a}{L} \right)^{(d-4)/3}, \quad x = \frac{\xi}{L} \left(\frac{a}{L} \right)^{(d-4)/3}, \quad (46)$$

we obtain the scaling relation in analytical form:

$$\pm \frac{1}{x^2} = y - \frac{1}{y^2}, \quad (47)$$

where all coefficients are made equal to unity by redefinition of the scales for ξ_{1D} and ξ . Relations (46), (47) contain the atomic scale a , as was expected from the nonrenormalizability of the theory (Section 1).

According to (46), (47), the role of the scaling parameter is played by quantity y instead of ξ_{1D}/L ; the L dependence of y is analogous to Fig. 1; i.e., all curves corresponding to $\tau > 0$ and $\tau < 0$ can be reduced to two universal ones by the scale transformation. The transition point corresponds to $y = 1$, since

$$\frac{\xi_{1D}}{L} \sim \left(\frac{L}{a} \right)^{(d-4)/3}, \quad \tau = 0 \quad (48)$$

and the critical point cannot be fixed by the condition $\xi_{1D}/L = \text{const}$.

5.2. Four-Dimensional Case

In the case $d = 4$, we analogously have

$$I_2(m) = \begin{cases} -c_4 m^2 \ln \frac{\Lambda}{m} + O(1), & m \gtrsim L^{-1} \\ -c_4 m^2 \ln(\Lambda L) + O(1), & m \lesssim L^{-1}; \end{cases} \quad (49)$$

i.e., the two results differ by $\ln(mL)$, which reduces to a double-logarithmic quantity in the actual region (see below). Neglecting such quantities, we can also obtain

scaling for $d = 4$. The self-consistency equation has the form

$$\tau \Lambda^2 = \frac{1}{2mL^3} - c_4 m^2 \ln \frac{\Lambda}{m} \quad (50)$$

and after changing to ξ and ξ_{1D}

$$\pm \frac{c_4}{\xi^2} \ln \left(\frac{\xi}{a} \right) = \frac{\xi_{1D}}{2L^3} - \frac{c_4}{\xi_{1D}^2} \ln \left(\frac{\xi_{1D}}{a} \right). \quad (51)$$

The scaling relation (47) is obtained in variables

$$y = \frac{\xi_{1D}}{L} \left[\ln \left(\frac{L}{a} \right) \right]^{-1/3}, \quad (52)$$

$$x = \frac{\xi}{[\ln(\xi/a)]^{1/2}} \frac{[\ln(L/a)]^{1/6}}{L},$$

i.e., scaling parameter y is logarithmically modified in comparison with ξ_{1D}/L and should be considered as a function of ‘‘modified length’’ $\mu(L) = L[\ln(L/a)]^{-1/6}$; then all dependences become analogous to Fig. 1 and a change in scale for $\mu(L)$ allows reducing them to two universal curves for $\tau > 0$ and $\tau < 0$. The critical point corresponds to $y = \text{const}$, since

$$\frac{\xi_{1D}}{L} \sim \left(\ln \frac{L}{a} \right)^{1/3}, \quad \tau = 0; \quad (53)$$

i.e., parameter ξ_{1D}/L increases logarithmically in the transition point.

5.3. Modified Scaling for $d = 4 - \epsilon$

From the methodical point of view, it is interesting to derive the modified scaling for $d = 4 - \epsilon$; in this case, the sum $I_2(m)$ converges formally at the upper limit, but this convergence is slow and finiteness of Λ gives the essential effect. Analogously to (49) we have

$$I_2(m) = \begin{cases} -c_4 m^2 \frac{m^{-\epsilon} - \Lambda^{-\epsilon}}{\epsilon}, & m \gtrsim L^{-1} \\ -c_4 m^2 \frac{L^{\epsilon} - \Lambda^{-\epsilon}}{\epsilon}, & m \lesssim L^{-1} \end{cases} \quad (54)$$

and the scaling relation (47) is obtained in variables

$$y = \frac{\xi_{1D}}{L} \left[\frac{\epsilon}{1 - (L/a)^{-\epsilon}} \right]^{1/3}, \quad (55)$$

$$x = \frac{\epsilon^{1/3} (\xi/a) [1 - (L/a)^{-\epsilon}]^{1/6}}{[(\xi/a)^{\epsilon} - 1]^{1/2} (L/a)^{1-\epsilon/2}}.$$

Once again we have the modified scaling parameter y and modified length $\mu(L) = L^{1-\epsilon/2} [1 - (L/a)^{-\epsilon}]^{-1/6}$, in

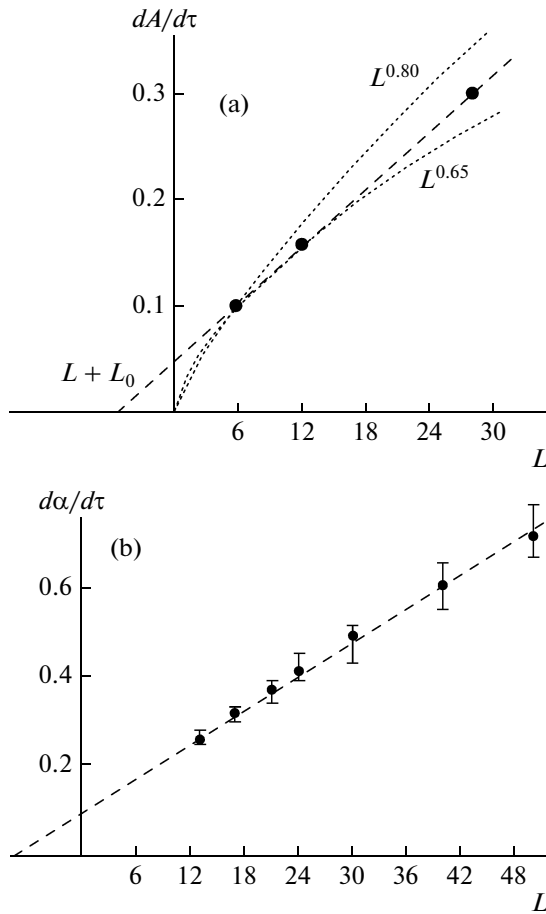


Fig. 7. Fitting by dependence $(L + L_0)$ (dashed line) for numerical data, based on the level statistics: (a) Data by Zharekeshev and Kramer [27]. The points correspond to the average derivatives of the scaling parameter A (arbitrary units), determined from Fig. 4 of [27] in the interval $16 < W < 17$; a statistical error related with each point can be estimated very conservatively (see Table in [2]) due to the irregular character of curves given in the indicated figure; uncertainty allowed by the authors themselves corresponds to the gap between dependences $L^{0.80}$ and $L^{0.65}$, determining the upper and lower bound of the result for the critical exponent, $\nu = 1.40 \pm 0.15$. (b) Data obtained by Schreiber' group [43]; the points correspond to the derivative of the scaling parameter α (arbitrary units) determined by the slope of solid lines in the inset of Fig. 3 in [43]; their uncertainty is obtained by variation of the slope allowed by the size of experimental points.

terms of which the dependences of Fig. 1 are recovered. In the critical point we have $y = 1$ and

$$\begin{aligned} \frac{\xi_{1D}}{L} &= \left[\frac{1 - (L/a)^{-\epsilon}}{\epsilon} \right]^{1/3} \\ &= \begin{cases} [\ln(L/a)]^{1/3}, & \ln(L/a) \lesssim 1/\epsilon \\ (1/\epsilon)^{1/3}, & \ln(L/a) \gtrsim 1/\epsilon; \end{cases} \end{aligned} \quad (56)$$

i.e., parameter ξ_{1D}/L increases logarithmically up to the large length scale $L_0 \sim a \exp\{\text{const}/\epsilon\}$ and then is saturated at the constant value. Such scaling is useful

as an alternative treatment for $d = 3$ in order to investigate systematic errors related to the possible existence of the large length scale. In this case, parameter a in fact corresponds to L_0 and can be essentially different from the lattice constant; it should be adjusted from the condition of best scaling quality. There is no need to be bound by Eq. (47), which is valid for small ϵ ; it is more reasonable to determine the relation $y = F(x)$ empirically. As for expressions (55), their extrapolation to $\epsilon = 1$ does not present any problem, since for $L, \xi \gg a$ the modified scaling safely reduces to the usual one (see Eq. (4)). In fact, it is identical to Eq. (4) if no large scale L_0 is present. However, in the presence of large length L_0 , such scaling is more adequate than (4).

6. CONCLUSIONS

The above analysis allows us to conclude that the Vollhardt-Wölfle theory has no significant contradictions to numerical results on the level of raw data. The different critical behavior usually reported in numerical papers originates from the fact that some time ago, the purely “experimental” approach to the problem was rejected and replaced by phenomenological analysis, which is practically hopeless in the corresponding region. In particular, dependence $L + L_0$ with $L_0 > 0$ is interpreted as $L^{1/\nu}$ with $\nu > 1$.

We have limited our discussion to the widespread variant of finite-size scaling, based on application of auxiliary quasi-1D systems. Apart from it, another algorithms are used, based on level statistics [20], conductance distribution, mean conductance, etc. [1]. The scaling curves calculated above are not universal and cannot be used for comparison with such results. Scaling for higher dimensions is also not universal: for example, another behavior in the critical point is expected for the Thouless parameter differing from (48), (53) [40]. The only exclusion is result (40), which remains unchanged in all cases. Indeed, this result can be obtained from the general arguments based on the Wilson renormalization group [2]; the exponents $\omega_1, \omega_2, \nu_1, \nu_2, \dots$ are determined by the scaling dimensions of irrelevant parameters and are hence universal. Correspondingly, result (41) is unchanged, which explains the origin of the effective values $\nu > 1$ (Fig. 7).

Figure 7a can be considered as a benchmark illustration, corresponding to most of the numerical papers. Indeed, there is an overall consensus that data for $L \lesssim 5$ fall out of the scaling pattern and should be discarded; large systems with $L \gtrsim 30$ are hardly ever used; the error corridor between dependences $L^{0.80}$ and $L^{0.65}$ corresponds to the typical accuracy of numerical papers. Figure 7b illustrates one of the rare papers treating systems of record size [43].⁹

⁹ The rare example of high-precision data is illustrated by the colored Fig. 8 in the online version of the paper [44].

Our final remark is as follows. Even if subsequent investigations reveal that the Vollhardt and Wölfle theory is not exact, nevertheless no confidence can be given to the present-day estimates of the exponent ν [17–31]. Figure 6 clearly demonstrates that values $\nu \approx 1.6$ and $\nu = 1$ are equally compatible with the raw data, and hence the treatment procedure is extremely ambiguous.

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