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Shape of crossover between mean-field and asymptotic critical behavior in a three-dimensional Ising lattice [1,2]

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Abstract

Recent numerical studies of the susceptibility of the three-dimensional Ising model with various interaction ranges have been analyzed with a crossover model based on renormalization-group matching theory. It is shown that the model yields an accurate description of the crossover function for the susceptibility. © 1999 Published by Elsevier Science B.V. All rights reserved.

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Recently, an accurate numerical study of the crossover from asymptotic (Ising-like) critical behavior to classical (mean-field) behavior has been performed both for two-dimensional [1,2] and three-dimensional [3] Ising systems in zero field on either side of the critical temperature with a variety of interaction ranges. It is the objective of the present work to analyze these numerical results within the framework of a crossover theory that is based on renormalization-group matching and that has already successfully been applied to the description of crossover in several experimental systems [4,5].

Qualitatively, the crossover is ruled by the parameter t/G where $t=(T-T_c)/T_c$ is the reduced temperature distance to the critical temperature T_c and G the Ginzburg number [6]. The Ginzburg number depends on the normalized interaction range R as

$$G = G_0 R^{-2d/(4-d)}, \tag{1}$$

where d is the dimensionality of space and G_0 a constant. Hence, for $d=3$ the crossover occurs as a function of tR^6. Asymptotic critical behavior takes place for $tR^6 \ll 1$ and classical behavior is expected for $tR^6 \gg 1$. In real fluids the crossover is never completed in the critical domain (where $t \ll 1$),

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since the range of interaction is of the same order of magnitude as the distance between molecules $(R \simeq 1)$ [4]. A new Monte-Carlo algorithm, developed by Luijten and Blöte [7], offers the advantage that the ratio t/G can be tuned over more than eight orders of magnitude allowing one to cover the full crossover region in three-dimensional spin models [3].

A sensitive description of crossover behavior is obtained from an analysis of the effective critical exponent of the susceptibility (the third derivative of the free energy), defined as

$$\gamma_{\text{eff}}^{\pm} \equiv -\, \mathrm{d}\ln \hat{\chi} / \mathrm{d}\ln|t|, \tag{2}$$

where the scaled susceptibility $\hat{\chi} = k_{\mathrm{B}} T_{\mathrm{c}}(R)(\partial m/\partial h)_T$, k_{B} the Boltzmann constant, m the order parameter, h the ordering field, and where the '$+$' sign applies for $T > T_{\mathrm{c}}$, and the '$-$' sign for $T < T_{\mathrm{c}}$. As is seen from Figs. 1 and 2, the variation of $\gamma_{\text{eff}}^{\pm}$ reproduces the Ising asymptotic critical behavior $(\gamma_{\text{eff}}^{\pm} \simeq 1.24)$ at $tR^6 \ll 1$ as well as the mean-field asymptote $(\gamma_{\text{eff}}^{\pm} = \gamma_{\mathrm{MF}} = 1)$ at $tR^6 \gg 1$. Apparently, all data would seem to collapse onto a universal function of the reduced variable tR^6 as predicted by a field-theoretical treatment [8,9] and by the ε-expansion [10]. However, as was noted in Ref. [3], a more careful look at the data reveals a remarkable discrepancy between the theoretical calculations [8–12] and the simulation results. Namely, the shape of the crossover is sharper than predicted by the theory [11,12], especially for short ranges of interaction. We will show that this discrepancy is related to the findings of Refs. [4,5], where it was shown that there is a fundamental problem in describing the crossover of $\gamma_{\text{eff}}^{\pm}$ by a universal function which contains only a single crossover parameter $G \propto R^{-6}$.

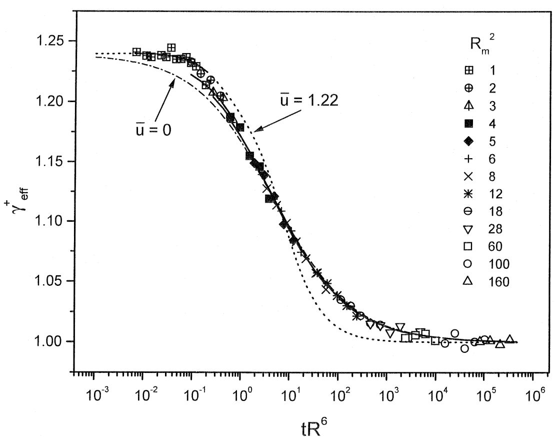

Fig. 1. The effective susceptibility exponent γ_{eff}^{+} above T_{c}. The symbols indicate numerical simulation data [3]. The solid curves represent values calculated from Eq. (5). The dashed-dotted curve corresponds to the limit $\bar{u} \to 0$. The dotted curve is a continuation of the crossover curve for $\bar{u} = 1.22$. For clarity, the error bars have been omitted; they are all of the order of 0.004.

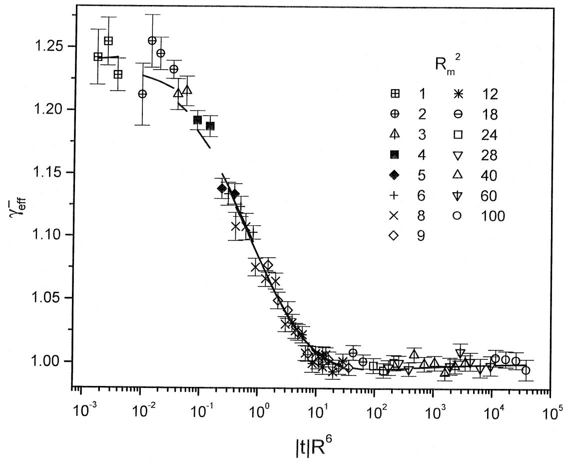

Fig. 2. The effective susceptibility exponent γ_{eff}^{-} below T_{c}. The symbols indicate numerical simulation data [3]. The solid curves represent values calculated from the renormalization-group matching crossover model.

In zero-ordering field above T_{c} the susceptibility asymptotically close to the critical point behaves as

$$\chi = \Gamma_0 t^{-\gamma}\left(1 + \Gamma_1 t^{\Delta_{\mathrm{s}}} + \Gamma_2 t^{2\Delta_{\mathrm{s}}} + a_1 t + \dots\right), \tag{3}$$

where $\gamma = 1.239 \pm 0.002$ (see, e.g., Refs. [13,14] and references therein) and $\Delta_{\mathrm{s}} = 0.504 \pm 0.008$ [15] are universal Ising critical exponents, and where Γ_0, Γ_1, Γ_2, and a_1 are system-dependent amplitudes. Expansion (3) is called the Wegner series [16].

In a universal single-parameter crossover theory [8–10], the Ginzburg number is responsible both for the range of validity of the mean-field approximation and for the convergence of the Wegner series (3). However, it is known [17–19], that the sign of the first Wegner correction amplitude Γ_1 depends on the difference $u - u^*$, where u is the scaled coupling constant and $u^* = 0.472$ is the universal coupling constant at the Ising fixed point [20]. Moreover, Liu and Fisher [18] concluded that the three-dimensional nearest-neighbor Ising model has a negative leading Wegner correction amplitude Γ_1, so that $\gamma_{\rm eff}^{\pm}$ asymptotically approaches $\gamma \simeq 1.24$ from above. Therefore, since the coupling constant itself depends on the interaction range, the shape of $\gamma_{\rm eff}^{\pm}$ cannot be represented by a universal function of the Ginzburg number, since G is not proportional to the difference $u-u^*$.

In this paper we therefore present an analysis of the numerical data for $\gamma_{\rm eff}^{\pm}$ [3] in terms of a crossover model based on renormalization-group matching for the free-energy density [17,19,21]. This model contains two crossover parameters $\bar{u}=u/u^*$ and Λ (a dimensionless cut-off wave number), and two rescaled amplitudes c_t and c_ρ related to the coefficients of the local density of the classical Landau–Ginzburg free energy ΔA:

$$\frac{v_0}{k_{\rm B}T}\frac{{\rm d}(\Delta A)}{{\rm d}V} = \tfrac{1}{2}a_0\tau\varphi^2 + \frac{1}{4!}u_0\varphi^4 + \tfrac{1}{2}c_0(\nabla\varphi)^2$$

$$= \tfrac{1}{2}c_t\tau M^2 + \frac{1}{4!}u^*\bar{u}\Lambda M^4 + \tfrac{1}{2}(\tilde{\nabla}M)^2, \tag{4}$$

with $\tau=(T-T_{\rm c})/T$, $M=c_\rho\varphi=(a_0/c_t)^{1/2}\varphi$, $a_0=c_\rho^2 c_t$, $u_0=u^*\bar{u}\Lambda c_\rho^4$, $c_0=c_\rho^2 v_0^{2/3}$, and $\tilde{\nabla}=v_0^{1/3}\nabla$. The average molecular volume v_0 and the prefactor $v_0/k_{\rm B}T$ are introduced to make the free-energy density and all the coefficients dimensionless. The inverse crossover susceptibility $\chi^{-1} = \left(\partial^2\Delta\tilde{A}/\partial M^2\right)_\tau$, where $\Delta\tilde{A}$ is the crossover (renormalized) free-energy density, in zero field above $T_{\rm c}$ reads [4]

$$\chi^{-1} = c_\rho^2 c_t \tau Y^{(\gamma-1)/\Delta_{\rm s}}(1+y) \tag{5}$$

with

$$y = \frac{u^*\nu}{2\Delta_{\rm s}}\left\{2\left(\frac{\kappa}{\Lambda}\right)^2\left[1+\left(\frac{\Lambda}{\kappa}\right)^2\right]\right.$$

$$\left.\times\left[\frac{\nu}{\Delta_{\rm s}}+\frac{(1-\bar{u})Y}{1-(1-\bar{u})Y}\right]-\frac{2\nu-1}{\Delta_{\rm s}}\right\}^{-1}, \tag{6}$$

where $\nu\simeq 0.630$ [15,22] is the critical exponent of the asymptotic power law for the correlation length ξ [4]. Note that $\chi^{-1}=(T_{\rm c}/T)\hat{\chi}^{-1}$ and the relation between $\gamma_{\rm eff}\equiv -\,{\rm d}\ln\chi/{\rm d}\ln|\tau|$ and $\gamma_{\rm eff}^{\pm}$, given by Eq. (2), is $\gamma_{\rm eff}^{\pm}=\gamma_{\rm eff}+(1-\gamma_{\rm eff})\tau$, both above and below the critical temperature. The crossover function Y is defined by

$$1-(1-\bar{u})Y = \bar{u}\left[1+\left(\frac{\Lambda}{\kappa}\right)^2\right]^{1/2} Y^{\nu/\Delta_{\rm s}} \tag{7}$$

and is to be found numerically. The parameter κ in Eq. (7) is inversely proportional to the fluctuation-induced portion of the correlation length and serves as a measure of the distance to the critical point. In zero field above $T_{\rm c}$ the expression for κ^2 reads:

$$\kappa^2 = c_t\frac{T}{T_{\rm c}}\tau Y^{(2\nu-1)/\Delta_{\rm s}} = c_t t Y^{(2\nu-1)/\Delta_{\rm s}}. \tag{8}$$

We modified the original expression for κ^2, given by Eq. (3) in Ref. [4], by introducing the non-asymptotic factor $T/T_{\rm c}$ in Eq. (8) so that κ^2 becomes infinite at $T\to\infty$ [23]. Asymptotically close to the critical point $(\Lambda/\kappa \gg 1)$, the following expression is obtained for the first correction amplitude Γ_1 in Eq. (3):

$$\Gamma_1 = g_1\left(\frac{\sqrt{c_t}}{\bar{u}\Lambda}\right)^{2\Delta_{\rm s}}(1-\bar{u}), \tag{9}$$

where $g_1\simeq 0.62$ is a universal constant [21].

In the approximation of an infinite cut-off $\Lambda\to\infty$, which physically means neglecting the discrete structure of matter, $\bar{u}=u_0c_t^2/(u^*\Lambda a_0^2)\to 0$ and the two crossover parameters $\bar{u}$ and Λ in the crossover equations collapse into a single one, $\bar{u}\Lambda$, which is related to the Ginzburg number G by [21]

$$G = g_0\frac{(\bar{u}\Lambda)^2}{c_t} = g_0\frac{u_0^2 v_0^2}{(u^*)^2 a_0^4\bar{\xi}_0^6}, \tag{10}$$

where $g_0\simeq 0.028$ is a universal constant [21] and $\bar{\xi}_0 = v_0^{1/3}c_t^{-1/2}=(c_0/a_0)^{1/2}$ is the mean-field amplitude of the power law for the correlation length. Note that the Ginzburg number does not depend explicitly on the cut-off Λ or on $\bar{u}$. This single-parameter crossover, i.e., the crossover for $\bar{u}=0$, is universal and is indicated in Fig. 1 by a dashed-dotted curve. This simplified description of the crossover is equivalent to the results of Bagnuls and Bervillier [9] and of Belyakov and Kiselev [10].

In the simulations [3], each spin interacts equally with its z neighbors lying within a distance $R_{\rm m}$ on a three-dimensional cubic lattice. The effective range of interaction R is then defined as $R^2 = z^{-1}\sum_{j\neq i}|\boldsymbol{r}_i - \boldsymbol{r}_j|^2$ with $|\boldsymbol{r}_i - \boldsymbol{r}_j| \leq R_{\rm m}$ [1]. We have approximated the relation between R and $R_{\rm m}$ by $R^2 = \frac{3}{5}R_{\rm m}^2(1+\frac{2}{3}R_{\rm m}^{-2})$, as indicated in the insert in Fig. 3. In order to compare the numerical results to the theoretical prediction Eq. (5), we need the range dependence of the parameters c_t and $\bar{u}$. Indeed, the asymptotic R dependence of $\bar{u}$ follows directly from simple scaling arguments [1], $\bar{u} = \bar{u}_0 R^{-4}$, and c_t varies as its square root, $c_t = c_{t0} R^{-2}$. For a three-dimensional simple cubic lattice, $\Lambda = \pi$ [18,24], and we obtain for the Ginzburg number

$$G = G_0 R^{-6} = 0.28\left(\bar{u}_0^2/c_{t0}^4\right)c_t^3 = 0.28\left(\bar{u}_0^2/c_{t0}\right)R^{-6}. \tag{11}$$

The non-universal parameters c_{t0} and $\bar{u}_0$ have to be determined from a least-squares fit to the numerical data for $\gamma_{\rm eff}^+$, which yielded $c_{t0} = 1.72$ and $\bar{u}_0 = 1.22$ and hence $G_0 \approx 0.24$. The solid lines in Fig. 1 indicate the corresponding theoretical curves. It should be noted that these curves are calculated for each value of R_m separately; the piecewise continuous character of this description directly reflects the fact that the crossover cannot be described by a universal single-parameter function. Indeed, Fig. 1 also shows two attempts to describe the data in terms of such a function. The dash-dotted line corresponds to the limit $\bar{u} \to 0$, whereas the dotted curve corresponds to $\bar{u}_0 = 1.22$ and $\Lambda = \pi$ (a continuation of the theoretical curve for $R = 1$). We see that the actual crossover lies between these two bounding curves, with $\bar{u} \simeq 0$ for large R and $\bar{u} \simeq 1.2$ for $R = 1$. Thus, it is clearly seen that without including the R dependence of $\bar{u}$ it is impossible to describe data for short interaction ranges $R_{\rm m}^2 \leq 5$. The dependence of $\bar{u}$ on R is shown in Fig. 3. The two adjustable parameters c_{t0} and $\bar{u}_0$ are strongly correlated and if one of them is fixed at a predicted value, the quality of the description remains the same. We hence tried to fit the data while keeping c_{t0} fixed at the theoretically predicted value $c_{t0} = 2d = 6$ [25,26]. In this case a fit of the same quality is obtained with $\bar{u}_0 = 1.22$, provided that $\Lambda \simeq 2\pi$. The value of $G_0 \approx 0.24$ then remains unchanged.

To describe the data below the critical temperature, a connection between M and τ in zero field is to be found from the condition $(\partial\Delta\tilde{A}/\partial M)_\tau = 0$. The relation between M and τ appears to be implicit and χ as a function of τ cannot be expressed in an explicit form either. Of course, the parameters c_{t0} and $\bar{u}_0$ should be the same as for $T > T_{\rm c}$ and we hence kept them fixed at the above-mentioned values. However, the parameter G_0 appearing in Eq. (11) will take a different value. We took this into account by introducing a factor G_0^+/G_0^- into the temperature scale: $t \to t\cdot(G_0^+/G_0^-)$. Fig. 2 shows the results for $T < T_{\rm c}$, where the factor G_0^+/G_0^- was included as an adjustable parameter. Our estimate $G_0^-/G_0^+ = 2.58$ must be compared with the theoretical result $G_0^-/G_0^+ = 3.125$ [27]. Interestingly, $\gamma_{\rm eff}^-$ clearly shows a minimum around $|t|R^6 \sim 10^2$. This corroborates the non-monotonic character of the crossover of $\gamma_{\rm eff}^-$, earlier observed for the two-dimensional Ising lattice [2], where the effect is much more pronounced. We note that already in Ref. [28] a field-theoretic calculation of the crossover in the low-temperature regime has been given (in the limit $\bar{u} \to 0$), but only recently this has been extended to cover the full crossover region [29]. Actually, also here a non-monotonicity in $\gamma_{\rm eff}^-$ has been observed.

In summary, we remark that although in general the theory contains two crossover parameters $\bar{u}$ and Λ, only one parameter ($\bar{u}$) changes with the range of interaction. However, this does not mean that the crossover is a universal function of tR^6. Indeed, the

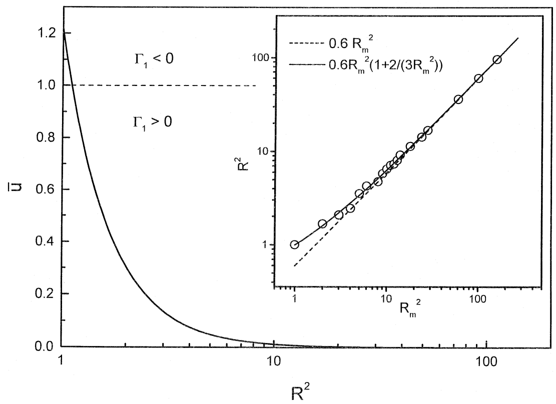

Fig. 3. Dependence of the normalized coupling constant $\bar{u}$ on the normalized interaction range R. Note that $\bar{u}$ becomes larger than unity for very short interaction ranges. Insert: Effective range of interaction R (open circles) plotted as a function of $R_{\rm m}$. The solid line corresponds to the approximation mentioned in the text and the dashed line represents the asymptotic behavior for large R.

effective range of interaction R affects the behavior of $\gamma_{\rm eff}^{\pm}$ in a twofold way: through the Ginzburg number, which is proportional to c_t^3, and through the first Wegner correction, with an amplitude Γ_1 that is proportional to $(1-\bar{u})$ [Eq. (9)]. Hence, there is no way to describe the data for short interaction ranges without allowing for $\bar{u}$ to become larger than unity and correspondingly Γ_1 to change its sign between $R_{\rm m}=2$ and $R_{\rm m}=1$ as indicated in Fig. 3. In previous publications we have shown that Eq. (5), derived from renormalization-group matching, gives an excellent representation of the experimentally observed crossover behavior in simple and complex fluids [4,5,30]. From the evidence presented in this paper, we conclude that the same crossover model also yields a quantitative description of the crossover critical behavior of a three-dimensional Ising lattice.

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