Shape of Crossover Between Mean-Field and Asymptotic Critical Behavior in a Three-Dimensional Ising Lattice

M. A. Anisimov, E. Luijten, V. A. Agayan, J. V. Sengers, and K. Binder

1Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742, USA
2Department of Chemical Engineering, University of Maryland, College Park, MD 20742, USA
3Max-Planck-Institut für Polymerforschung, Postfach 3148, D-55021, Mainz, Germany
4Institut für Physik, WA 331, Johannes Gutenberg-Universität, D-55099 Mainz, Germany

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.

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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 [4] 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].

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 [3]. The Ginzburg number depends on the normalized interaction range $R$ as

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

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 $t \ll 1$), since the range of interaction is of the same order of magnitude as the distance between molecules ($R \approx 1$) [4]. A new Monte-Carlo algorithm, developed by Luijten and Blöte [5], 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 [4].

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

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

where the scaled susceptibility $\chi = k_B T_c (\partial m/\partial h)_T$, $k_B$ the Boltzmann constant, $m$ the order parameter, $h$ the ordering field, and where the “+” sign applies for $T > T_c$, and the “−” sign for $T < T_c$. 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 ($\gamma_{\text{eff}}^{\pm} = \gamma_{\text{MF}} = 1$) 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 [4] and by the $\varepsilon$-expansion [6]. However, as was noted in Ref. [7], a more careful look at the data reveals a remarkable discrepancy between the theoretical calculations [6,12] 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 $G \propto R^{-6}$.

In zero-ordering field above $T_c$ the susceptibility asymptotically close to the critical point behaves as

$$\chi = \Gamma_0 t^{-\gamma} \left(1 + \Gamma_1 t^{\Delta_+} + \Gamma_2 t^{2\Delta_+} + a_1 t + \ldots\right) ,$$

where

$\gamma \equiv 1$,
where $\gamma = 1.239 \pm 0.002$ (see, e.g., Refs. [13,14] and references therein) and $\Delta_s = 0.504 \pm 0.008$ [15] are universal Ising critical exponents, and where $\Gamma_0$, $\Gamma_1$, $\Gamma_2$, and $a_1$ are system-dependent amplitudes. Expansion [6] is called the Wegner series [6].

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 [17–19,4] that the sign of the first Wegner correction amplitude $\Gamma_1$ 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 [21]. Moreover, Liu and Fisher [15] concluded that the three-dimensional nearest-neighbor Ising model has a negative leading Wegner correction amplitude $\Gamma_1$, so that $\gamma_{\text{eff}}^+ - \gamma_{\text{eff}}^-$ asymptotically approaches $\gamma \approx 1.24$ from above. Therefore, since the coupling constant itself depends on the interaction range, the shape of $\gamma_{\text{eff}}$ 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 $\gamma_{\text{eff}}^\pm$ [8] in terms of a crossover model based on renormalization-group matching for the free-energy density [17,18,22]. This model contains two crossover parameters $\bar{u} = u/u^*$ and $\Lambda$ (a dimensionless cutoff wave number), and two rescaled amplitudes $c_t$ and $c_\rho$ related to the coefficients of the local density of the classical Landau–Ginzburg free energy $\Delta A$:

$$\frac{v_0}{k_B T} \frac{d(\Delta A)}{dV} = \frac{1}{2} a_0 \varphi^2 + \frac{1}{4!} a_0 \varphi^4 + \frac{1}{2} c_3 (\nabla \varphi)^2$$

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

with $\tau = (T - T_c)/T$, $M = c_\rho \varphi = (a_0/c_t)^{1/2} \varphi$, $a_0 = c_0^2 c_t$, $v_0 = u^* \bar{u} \Delta \rho_0^4$, $c_0 = c_0^2 v_0^{2/3}$, and $\bar{v} = v_0^{1/3} \nabla$. The average molecular volume $v_0$ and the prefactor $v_0/k_BT$ are introduced to make the free-energy density and all the coefficients dimensionless. The inverse crossover susceptibility $\chi^{-1} = (\partial^2 \Delta \hat{A}/\partial M^2)_\tau$, where $\Delta \hat{A}$ is the crossover (renormalized) free-energy density, in zero field above $T_c$ reads [4]

$$\chi^{-1} = c_t^2 c_t \tau Y^{(\gamma - 1)/\Delta_s} (1 + y)$$

with

$$y = \frac{u^* \nu}{2 \Delta_s} \left\{ 2 \left( \frac{\kappa}{\Lambda} \right)^2 \left[ 1 + \left( \frac{\Lambda}{\kappa} \right)^2 \right] \left[ \frac{(1 - \bar{u}) Y}{\Delta_s} - \frac{2 \nu - 1}{\Delta_s} \right] - \frac{1}{\Delta_s} \right\},$$

where $\nu \approx 0.630$ [13,22] is the critical exponent of the asymptotic power law for the correlation length $\xi$ [4]. Note that $\chi^{-1} = (T_c/T) \chi^{-1}$ and the relation between $\gamma_{\text{eff}} = -d \ln \chi / d \ln |\tau|$ and $\gamma_{\text{eff}}^\pm$ given by Eq. (2), is $\gamma_{\text{eff}}^\pm = \gamma_{\text{eff}} + (1 - \gamma_{\text{eff}}) \tau$, both above and below the critical temperature. The crossover function $Y$ is defined by

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

and is to be found numerically. The parameter $\kappa$ in Eq. (6) 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 $T_c$ the expression for $\kappa^2$ reads:

$$\kappa^2 = \frac{c_t}{T_c} \tau Y^{(2\nu - 1)/\Delta_s} = \frac{c_t Y^{(2\nu - 1)/\Delta_s}}{T_c}.$$

We modified the original expression for $\kappa^2$, given by Eq. (3) in [4], by introducing the non-asymptotic factor $T/T_c$ in Eq. (8) so that $\kappa^2$ 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 $\Gamma_1$ in Eq. (4):

$$\Gamma_1 = g_1 \left( \frac{\sqrt{c_t}}{u \Lambda} \right)^{2 \Delta_s} (1 - \bar{u}),$$

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

In the approximation of an infinite cutoff $\Lambda \to \infty$, which physically means neglecting the discrete structure of matter, $\bar{u} = u_0 c_t^2/(u^* \Delta \rho_0^2) \to 0$ and the two crossover parameters $\bar{u}$ and $\Lambda$ in the crossover equations collapse into a single one, $\bar{u} \Lambda$, which is related to the Ginzburg number $G$ by [21].
\[ G = g_0 \left( \frac{\bar{u}\Delta^2}{c_t} \right) = g_0 \frac{u_0^2}{(\bar{u}^*)^2} = \frac{u_0^2}{a_0^2 \zeta_0^6}, \]  
\hspace{1cm} (10)

where \( g_0 \approx 0.028 \) is a universal constant \( [21] \) and \( \zeta_0 = \frac{u_0^{1/3}}{c_t^{1/2}} = (c_0/\bar{u}_0)^{1/2} \) is the mean-field amplitude of the power law for the correlation length. Note that the Ginzburg number does not depend explicitly on the cutoff \( \Lambda \) 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 \( [11] \).

In the simulations \( [4] \), each spin interacts equally with its \( z \) neighbors lying within a distance \( R_m \) on a three-dimensional cubic lattice. The effective range of interaction \( R \) is then defined as \( R^2 = z^{-1} \sum_{j \neq i} |r_i - r_j|^2 \) with \( |r_i - r_j| \leq R_m \) \( [1] \). We have approximated the relation between \( R \) and \( R_m \) by \( R^2 = \frac{2}{3} R_m^2 (1 + \frac{2}{3} R_m^2) \), as indicated in the inset in Fig. 3. In order to compare the numerical results to the theoretical prediction Eq. \( (3) \), 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, \( c_t = c_0 R^{-2} \). For a three-dimensional simple cubic lattice, \( \Lambda = \pi [\bar{u}^4] \), and we obtain for the Ginzburg number

\[ G = G_0 R^{-6} = 0.28(\bar{u}_0^2/a_0^4) c_t^4 = 0.28(\bar{u}_0^2/c_0) R^{-6}. \]  
\hspace{1cm} (11)

The nonuniversal parameters \( c_0 \) and \( \bar{u}_0 \) have to be determined from a least-squares fit to the numerical data for \( \gamma_\text{eff}^+ \), which yielded \( c_0 = 1.72 \) and \( \bar{u}_0 = 1.22 \) and hence \( G_0 \approx 0.24 \). The solid lines in Fig. 1 indicate the corresponding single-parameter functions. 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 \( \bar{u} \approx 0 \) for large \( R \) and \( \bar{u} \approx 1.2 \) 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 \( R_m^2 \leq 5 \). The dependence of \( \bar{u} \) on \( R \) is shown in Fig. 3. The two adjustable parameters \( c_0 \) 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 \( c_0 \) fixed and \( \bar{u}_0 = 2d = 6 [18, 24] \). In this case a fit of the same quality is obtained with \( \bar{u}_0 = 1.22 \), provided that \( \Lambda \approx 2\pi \). The value of \( G_0 \approx 0.24 \) then remains unchanged.

To describe the data below the critical temperature, a connection between \( M \) and \( \tau \) in zero field is to be found from the condition \( \langle \partial \Delta A/\partial M \rangle_\tau = 0 \). The relation between \( M \) and \( \tau \) appears to be implicit and \( \chi \) as a function of \( \tau \) cannot be expressed in an explicit form either. Of course, the parameters \( c_0 \) and \( \bar{u}_0 \) should be the same as for \( T > T_c \) 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: \( t \to t (G_0^+ / G_0^-) \). Figure 2 shows the results for \( T < T_c \), 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 \( G_0^- / G_0^+ = 3.125 \) \( [22] \). Interestingly, \( \gamma_\text{eff}^+ \) clearly shows a minimum around \( |t| R^6 \approx 10^2 \). This corroborates the nonmonotonic character of the crossover of \( \gamma_\text{eff}^+ \) earlier observed for the two-dimensional Ising lattice \( [4] \), where the effect is much more pronounced. We note that already in Ref. \( [24] \) 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 \( [24] \). Actually, also here a nonmonotonicity in \( \gamma_\text{eff}^+ \) has been observed.

In summary, we remark that although in general the theory contains two crossover parameters \( \bar{u} \) and \( \Lambda \), only one parameter \( \bar{u} \) changes with the range of interaction. However, this does not mean that the crossover is a universal function of \( t R^6 \). Indeed, the effective range of interaction \( R \) affects the behavior of \( \gamma_\text{eff}^+ \) in a twofold way: through the Ginzburg number, which is proportional to \( c_t^4 \), and through the first Wegner correction, with an amplitude \( \Gamma_1 \) that is proportional to \( (1 - \bar{u}) \) \( [4, 11] \). 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 \( \Gamma_1 \) to change its sign between \( R_m = 2 \) and \( R_m = 1 \) as indicated in Fig. 3. In previous publications we have shown that Eq. \( (3) \), derived from renormalization-group matching, gives an excellent representation of the experimentally observed crossover behavior in simple and complex fluids \( [4,18,20] \). 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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FIG. 1. The effective susceptibility exponent $\gamma_{\text{eff}}^+$ 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 $\gamma_{\text{eff}}^-$ below $T_c$. The symbols indicate numerical simulation data [3]. The solid curves represent values calculated from the renormalization-group matching crossover model.
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 $R_m$. The solid line corresponds to the approximation mentioned in the text and the dashed line represents the asymptotic behavior for large $R$. 