Critical scaling to infinite temperature

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Three-dimensional Ising model ferromagnets on different lattices with nearest-neighbor interactions, and on simple-cubic lattices with equivalent interactions out to further neighbors, are studied numerically. The susceptibility data for all these systems are analyzed using the critical renormalization-group theory formalism over the entire temperature range above T_c with an appropriate choice of scaling variable and scaling expressions. Representative experimental data on a metallic ferromagnet (Ni) and an elementary fluid (Xe) are interpreted in the same manner so as to estimate effective coordination numbers.

I. INTRODUCTION

In the very extensive studies that have been devoted to critical phenomena, attention has understandably been mainly concentrated on the regime in the immediate neighborhood of the critical temperature; data are analyzed using the leading terms in the renormalization-group theory (RGT) formalism. It is widely considered that as correction terms proliferate outside this narrow "critical region," they always lead ultimately toward Gaussian fixed point mean-field-like behavior above a temperature T_g determined by the Ginzburg criterion.[1] This criterion expresses a crossover from a fluctuation-dominated critical regime to a high-temperature Landau regime. Sophisticated theoretical and numerical studies have been done on this crossover,[2–7] particularly in the context of long-range interactions. Experimental data on fluids, where effective interactions are expected to be long range, have been interpreted on this basis.[8–10]

Here we discuss from a different perspective numerical data on various three-dimensional (3D) Ising systems, in particular models where the interactions extend beyond nearest neighbor. We conclude that with appropriate observables and choice of scaling variable, for this family of models at least there is no need to invoke a crossover or the Ginzburg criterion. The data can be convincingly interpreted using the rigorous critical RGT formalism over the whole temperature range from T_c to infinity. Applying Occam's razor, this approach is more economical conceptually as it requires only the extended critical analysis but no separate analysis linked to a crossover.

We discuss representative experimental data on a ferromagnet and on a fluid, showing that they too can be analyzed in a transparent manner using the same approach and without invoking crossovers. We obtain quantitative estimates of the effective coordination number for the metallic ferromagnet Ni and for the elementary fluid Xe.

II. SCALING

Before RGT, it was already established[11–13] that in the fundamental scaling law for ferromagnetics, the response parameter is the "reduced" susceptibility (see Ref. 13 for definitions),

$$\chi(\beta) = \langle (m - \langle m \rangle)^2 \rangle = \sum_{i,j} \langle S_i \cdot S_j \rangle = \chi_T(\beta)/\chi_0(\beta), \quad (1)$$

where the thermodynamic susceptibility

$$\chi_T(\beta) \equiv [\partial m/\partial H]_{H \to 0} \quad (2)$$

is normalized by the free spin susceptibility $\chi_0(\beta) \propto \beta$. (As usual, we will set the interaction strength J to 1 and write $\beta \equiv 1/kT$.) The critical behavior is written[13–16]

$$\chi(\beta) \equiv T \chi_T(\beta) \propto \epsilon^{-\gamma}(1 + \cdots), \quad (3)$$

where ϵ is an appropriately normalized scaling variable depending linearly on $(T - T_c)$ close to T_c.

The thermodynamic ideal lattice gas analog to χ_T is the isothermal compressibility on the critical isochore $K_T = -(\partial V/\partial p)/V$, so by strict analogy to the ferromagnetic case the parameter that should be scaled[13] is the compressibility normalized by the ideal gas compressibility $\langle (N - \langle N \rangle)^2 \rangle / \langle N \rangle$, where N is the total number of particles, i.e.

$$T K_T \propto \epsilon^{-\gamma}(1 + \cdots). \quad (4)$$

Because the gas-liquid order parameter is a scalar, the fluid transition belongs to the Ising universality class.[17] Careful experimental measurements and analyses made over many years (see Ref. 10) have shown that the asymptotic fluid critical exponents are indeed those of the short-range Ising universality class. The real situation is, however, more complicated than in the magnetic case because of the departure from vapor-liquid symmetry in real fluids[10,18,19]; the fluid "susceptibility" is defined in Ref. 10.

In work based on the high-temperature series expansion (HTSE) theory, which was already firmly established in the 1950s, the critical scaling variable is taken to be either $\epsilon = \tau = [1 - \beta/\beta_c]$ or $\epsilon = [1 - \tanh(\beta)/\tanh(\beta_c)]$.[11,12,16] Appropriate high-temperature series are written rigorously as sums of terms where exact factors multiply successive powers of ϵ. However, since the introduction of RGT, scaling expressions are often written in terms of $\epsilon = t = [(T - T_c)/T_c]$. This is just the simplest linear convention, but other scaling variables including τ are just as legitimate as t in the region very close to T_c. (For instance, in the special case of the square lattice Ising model, an extremely sophisticated analysis uses $[1/\sinh(2\beta) - \sinh(2\beta)]/2$ as the scaling variable.[15]) In addition, τ has obvious practical advantages in the temperature region well above T_c because its high-temperature limit is 1 (and not infinity, as is the case for t).

Systematic analyses of high-temperature numerical data of nearest-neighbor and long-range interaction models in the Ising universality class[3,7,8,20] have been carried out with an effective temperature-dependent susceptibility exponent defined as

$$\gamma_t(t) = -\partial \log \chi_T(\beta)/\partial \log t \qquad (5)$$

following the phenomenological expression of Kouvel and Fisher.[21] In the high-temperature limit for any spin model, $\chi_T \to 1/T$ and $t \to T$, so $\gamma_t(t)$ will automatically tend to 1 at high temperatures. There will necessarily be a crossover at an intermediate temperature where $\gamma_t(t)$ passes from the critical γ to 1. However, far from criticality the appropriate choice of variables is vital. Thus if the reduced susceptibility parameter $\chi(\beta)$ rather than $\chi_T(\beta)$ had been used for the definition of $\gamma_t(t)$ in Ref. 3 and following work, the effective exponent would have tended to 0 at high temperature, not to 1.

The full formal RGT Wegner scaling expression is for $\chi(\tau)$ rather than $\chi_T(t)$; in the thermodynamic limit including confluent and analytic plus background corrections, it is written rigorously in terms of τ as[14,16,22,23]

$$\chi(\tau) = T\chi_T(\tau) = C_\chi \tau^{-\gamma}[1 + a_\chi \tau^\theta F_a(\tau) + b_\chi \tau F_b(\tau)$$
$$+ c_\chi \tau^{(1-\alpha+\gamma)} F_c(\tau) + d_\chi \tau^\gamma F_d(\tau)$$
$$+ a_{2,\chi} \tau^{\theta_2} F_2(\tau) + \cdots], \qquad (6)$$

where γ, α, the confluent correction exponents θ_i, and certain amplitude ratios are universal but the amplitudes themselves are not universal; the F_i are infinite analytic series in τ normalized to 1 at $\tau = 0$. Because $\tau \to 1$ as $T \to \infty$, these developments remain well behaved at all temperatures above T_c, whereas because t diverges as T, it is obviously very awkward to extend to high temperatures the analogous expression written in terms of t.

The temperature-dependent effective susceptibility exponent defined in terms of τ and $\chi(\tau)$ in Refs. 16 and 24–27 is

$$\gamma_{\text{eff}}(\tau) = -\partial \log \chi(\tau)/\partial \log(\tau) \qquad (7)$$

with the equivalence

$$\gamma_t = \gamma_{\text{eff}}(1 - \tau) + \tau. \qquad (8)$$

Very close to T_c, the two effective γ parameters are indistinguishable, but they have quite different properties as soon as the temperature difference increases. [Historically, it is of interest to note that the equation[11]

$$1/\chi_T = (1/C)T[1 - (T_c/T)]^\gamma f(T_c/T) \qquad (9)$$

cited explicitly by Kouvel and Fisher[21] to justify their analysis in the vicinity of T_c is precisely of the form of Eq. (6), with τ as the scaling variable.]

At first glance, the sets of infinite series of corrections in Eq. (6) appear rather forbidding. However, from inspection of $S = 1/2$ HTSE (see, for instance, Ref. 16), there are exact closure rules at infinite temperature : $C_\chi(1 + a_\chi + \cdots) \equiv 1$ and $\gamma_{\text{eff}}(1) \equiv z\beta_c$,[24] where z is the coordination number and the $(\cdots)$ represent the exact sum of all the higher-order terms in Eq. (6) evaluated with τ set equal to 1. It turns out that for the 3D Ising models, which we will discuss explicitly, over a wide

temperature region above T_c the leading (confluent) Wegner correction term dominates. As a convenient approximation, all the remaining terms can be collected into a single weak effective correction term $k_\chi \tau^{\lambda_\chi}$, giving a compact approximate expression that can be used to fit the data over the entire temperature range above T_c:

$$\chi(\tau)\tau^\gamma = C_\chi(1 + a_\chi \tau^\theta + k_\chi \tau^{\lambda_\chi}) \qquad (10)$$

so

$$\gamma_{\text{eff}}(\tau) = \gamma - (a_\chi \theta \tau^\theta + k_\chi \lambda_\chi \tau^{\lambda_\chi})/(1 + a_\chi \tau^\theta + k_\chi \tau^{\lambda_\chi}). \qquad (11)$$

The closure rules then become

$$C_\chi(1 + a_\chi + k_\chi) = 1 \qquad (12)$$

and

$$\gamma - (a_\chi \theta + k_\chi \lambda_\chi)C_\chi = z\beta_c. \qquad (13)$$

Once the strictly defined critical amplitudes C_χ and a_χ are estimated for any particular model from data at temperatures close to criticality, k_χ and λ_χ are fixed also from the closure conditions, so the entire temperature dependencies of $\chi(\tau)$ and $\gamma_{\text{eff}}(\tau)$ are determined. [An expansion of Eq. (10) to include further explicit Wegner terms is possible when HTSE data and higher-order correction exponent values are available.]

While not rigorous except in the limits $\tau \to 0$ and $\tau \to 1$, this ansatz as it stands already gives a representation of the true behavior of $\chi(\tau)$, which turns out to be accurate to the 10^{-3} level over the whole temperature range above T_c for all the models we have studied. If $\gamma_{\text{eff}}(\tau)$ is transposed to γ_t through Eq. (8), a crossover behavior results (see Fig. 4); similar data have been analyzed using an approximant containing an implicit crossover function.[6,9]

III. ISING MODEL ANALYSIS

The temperature-dependent susceptibility $\chi(\beta, L)$ was evaluated on diamond, sc, bcc, and fcc lattices with nearest-neighbor interactions, see Refs. 27–29, where the numerical techniques are described, and on sc lattices with equivalent interactions up to second, third, fourth, or fifth neighbor following Refs. 30, 3, and 25. The coordination numbers are $z = 4, 6, 8, 12, 18, 26, 32$, and 56, respectively. As all these models are in the 3D short-range interaction Ising universality class, in the analysis below the numerical values for the universal 3D Ising exponents were fixed at $\gamma = 1.2371$, $\theta = 0.50$, and $\nu = 0.630$.[31,32] The critical inverse temperatures β_c for the various models were evaluated from the present data using the Binder cumulant $g(\beta, L)$ and the parameter $W(\beta, L)$ introduced in Ref. 33. The β_c values obtained from the finite-size scaling analysis are in full agreement with previous estimates, in particular those of Ref. 5 for the equivalent interaction models. The raw normalized reduced susceptibilities $\chi(\tau, L)\tau^\gamma$ as a function of τ^θ for the $z26$ (nearest, second nearest, and third nearest equivalent neighbors) sc Ising model at different sizes L are shown as an example in Fig. 1. The envelope curve, which can be seen by inspection, corresponds to the thermodynamic limit (effectively infinite size) behavior. Data for each of the other models have a qualitatively similar appearance (see Ref. 27 for the nearest-neighbor sc model). The susceptibility
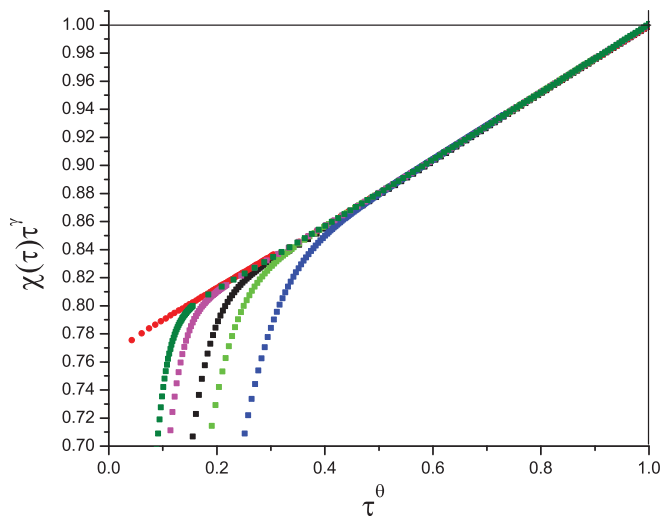
FIG. 1. (Color online) The raw normalized reduced susceptibility $\chi(\tau)\tau^\gamma$ as a function of τ^θ for the sc $z26$ (nearest, second nearest, and third nearest equivalent neighbors) Ising model. Lattice sizes $L = 32, 24, 16, 12,$ and 8 top to bottom (olive, pink, black, green, and blue). The $L > \xi(L,\beta)$ size-independent envelope behavior region can be seen for each curve by inspection. The envelope fit curve, with extrapolation, is in red.

results for infinite L (extrapolated for τ close to zero) for the various coordination numbers z are exhibited in Fig. 2 in the form of plots of $\chi(\tau)\tau^\gamma$ against τ^θ. The effective exponents $\gamma_{\rm eff}(\tau)$ derived from these data are shown in Fig. 3.

The critical parameter estimates $\beta_c(z)$, $C_\chi(z)$, and $a_\chi(z)$ and the approximate effective parameters $k_\chi(z)$ and $\lambda_\chi(z)$ are given in Table I. [The second correction term is always weak, so the values of $\lambda_\chi(z)$ are not precise as they depend very sensitively on the fit parameters chosen for the other variables.] All the models, including those with longer-range interactions, follow
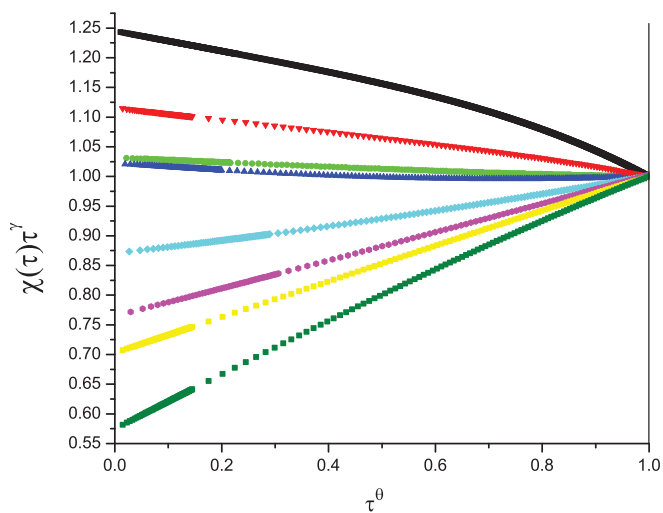

FIG. 2. (Color online) The normalized reduced susceptibility $\chi(\tau)\tau^\gamma$ as a function of τ^θ derived from data sets such as those shown in Fig. 1 for the diamond, sc, bcc, fcc, $z18$, $z26$, $z32$, and $z56$ sc Ising models, top to bottom (black, red, green, blue, cyan, pink, yellow, and olive). The critical exponents are taken to be $\gamma = 1.2371$ and $\theta = 0.50$.
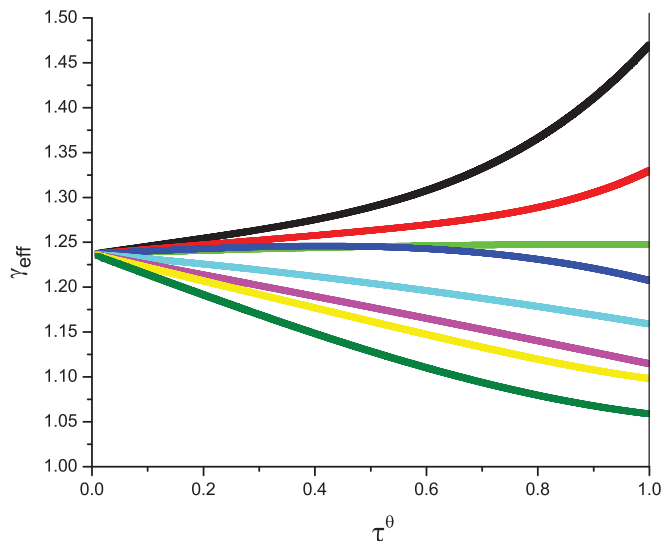

FIG. 3. (Color online) The effective exponent $\gamma_{\rm eff}(\tau)$ as a function of τ^θ derived from the data shown in Fig. 2 using Eq. (7) for the diamond, sc, bcc, fcc, $z18$, $z26$, $z32$, and $z56$ sc Ising models, top to bottom (black, red, green, blue, cyan, pink, yellow, and olive).

the critical scaling rules up to infinite temperature, with a gradual evolution of the critical amplitudes as z increases but without a trace of a crossover to mean-field behavior at high T. It is important to note that it is the coordination number z rather than the interaction range measured in terms of the nearest-neighbor distance that is the key parameter (with weak lattice structure effects); the diamond, sc, bcc, and fcc are all nearest-neighbor lattices, but they have significantly different values for C_χ and a_χ.

There seems no obvious reason to expect a breakdown in these rules however large the range of interactions as long as there is a cutoff so that the range remains finite; the correction amplitudes should continue to increase with increasing range. (If interactions fall off algebraically and sufficiently slowly, the models will leave the finite-range universality class.[34,35])

For comparison, the data of Fig. 3 translated appropriately are shown (Fig. 4) in the form of a γ_t against t/t_x where the normalization parameter is defined by $t_x = (a_{\chi,z})^{-1/\theta}$ as used in Ref. 9. It can be observed that there is no universality either in the position or the form of the individual curves.

TABLE I. Values of the fitting parameters for $\chi(\tau)$ in each of the models, as defined in Eq. (10)

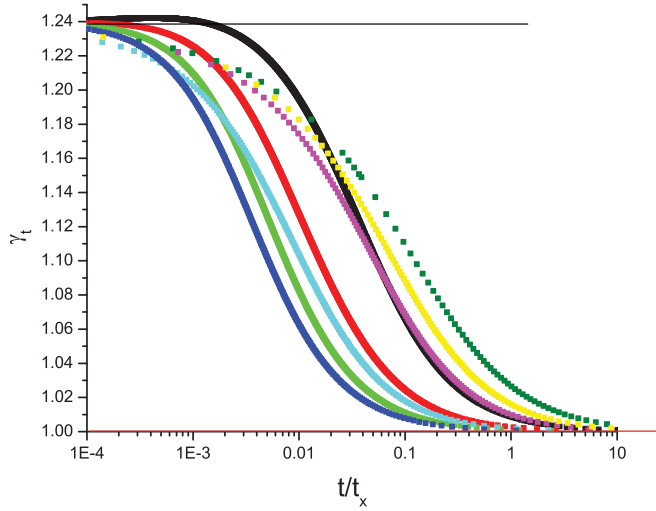| z	β_c	C_χ	a_χ	k_χ	λ_χ
4	0.3697	1.245	-0.1382	-0.059	2
6	0.221655	1.116	-0.0914	-0.0125	3
8	0.15737	1.038	-0.073	0.036	1.6
12	0.102067	1.022	-0.062	0.04	1.5
18	0.06442	0.871	0.111	0.038	0.9
26	0.0430385	0.765	0.302	0.009	1
32	0.0343267	0.703	0.428	-0.006	3
56	0.0189291	0.575	0.800	-0.06	1.5

FIG. 4. (Color online) The effective exponent γ_t as a function of t/t_x derived from the same susceptibility data, Fig. 2, using the definition Eq. (5), for the diamond, sc, bcc, fcc, $z18$, $z26$, $z32$, and $z56$ sc Ising models (black, red, green, blue, cyan, pink, yellow, and olive). t_x is defined following Ref. 9.

IV. EXPERIMENTAL DATA ANALYSIS

The present approach can be readily used to interpret experimental results. The venerable experimental data for the susceptibility of the ferromagnet Ni tabulated by Weiss and Forrer[36] and by Fallot[37] are exhibited in Fig. 5 in the same form as that used for the numerical data in Fig. 2. Here we consider Ni as an $S = 1/2$ Heisenberg local moment system and so use the Heisenberg exponent values $\gamma = 1.396$ and $\theta = 0.55$.[38] Following Fallot himself[37] and Ref. 39, we have subtracted out a small temperature-independent susceptibility term, which could well come from an orbital contribution
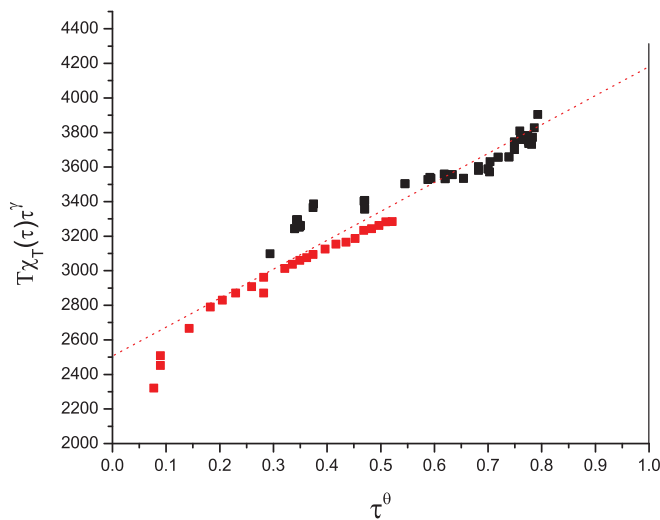

FIG. 5. (Color online) The normalized reduced susceptibility $T\chi_T(\tau)\tau^\gamma$ of Ni as a function of τ^θ with the Heisenberg exponents $\gamma = 1.349$ and $\theta = 0.55$. The experimental data and units are taken from Refs. 36 (red circles) and 37 (black squares). Following Refs. 37 and 39, a small temperature-independent term has been subtracted from the raw χ_T data.

(see Ref. 40 for the case of Co). As in the Ising models with higher coordination numbers shown in Fig. 2, the normalized reduced susceptibility increases almost linearly with τ^θ over the wide range of temperatures covered, which extends to $3T_c$, i.e. $\tau^\theta \sim 0.8$. The ratio between the asymptotic critical value of $\chi(\tau)\tau^\gamma$ and the estimated extrapolated infinite temperature value (equal to 1 for spin $1/2$ in the appropriate units) can be taken as a measure of the effective C_χ. For Ni, the observed ratio is about 0.60, or alternatively the correction amplitude $a_\chi \sim 0.65$.

As an example of a gas-liquid transition, we consider the susceptibility χ_T [defined as the derivative of the density by the chemical potential $\chi_T \equiv (\partial\rho/\partial\mu)_T$] of Xe on the critical isochore for the liquid-gas transition, for which results from careful experiments based on light-scattering techniques are tabulated in Ref. 41. In Fig. 6, these data are plotted in the form $T\chi_T\tau^\gamma$ against τ^θ, with the 3D Ising exponents. (It can be noted that the susceptibility χ_{NN} defined by Orkoulas *et al.*[19] in their analysis of the hard-core square-well fluid is $T\chi_T$; Orkoulas *et al.* also use τ as the scaling variable.) Again the figure shows an essentially linear increase of $T\chi_T\tau^\gamma$ with τ^θ just as in the numerical plots for the Ising models with large coordination numbers. The ratio of the critical limit to the extrapolated high-temperature limit is $C_\chi \sim 0.55$, or alternatively the correction amplitude $a_\chi \sim 0.75$. This value is broadly consistent with the values $a_\chi = 1.3(2)$ (Ref. 41) and $a_\chi = 1.08$ (Ref. 8) estimated from previous analyses based on the same data set but using different scaling rules. The complications associated with the asymmetry in the fluid phase diagram should be kept in mind, but this plot suggests that as in the magnetic case, even if fluid data were available to much higher τ within the present approach, there would be no need to invoke a crossover to mean-field-like behavior. In Fig. 7, the values of a_χ for the numerical models are plotted against z, and the effective values for Ni and for Xe are indicated by arrows. From this figure we can estimate the effective coordination number z for Ni and for Xe. To obtain a more quantitative estimate, the Ni experimental data should be compared to numerical results for Heisenberg spins on an
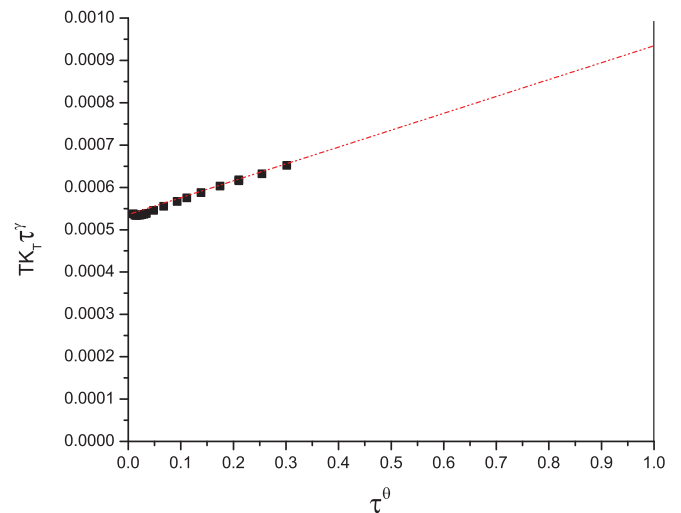

FIG. 6. (Color online) The normalized reduced compressibility $T K_T\tau^\gamma$ of Xe as a function of τ^θ. Experimental data and units taken from Ref. 41.
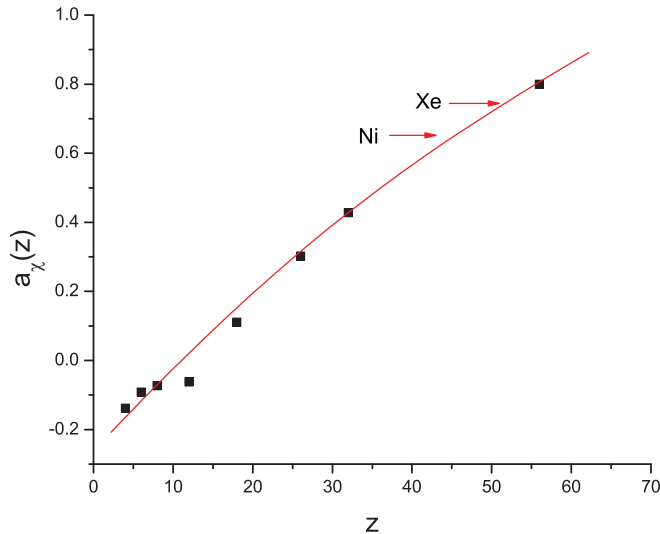
FIG. 7. (Color online) The effective critical correction amplitudes $a_\chi(z)$ for the Ising models as a function of coordination number z, Table I, plus points for Ni and Xe obtained from the plots of the experimental data in Figs. 5 and 6 (arrows).

fcc lattice for different z rather than for Ising spins on an sc lattice. From data comparing $\gamma(\tau)$ on Heisenberg spins on sc, bcc and fcc lattices,[24] it appears that the numerical $a_\chi(z)$ plot will be of similar form for Heisenberg spins as for Ising spins. One can then estimate that approximately $z \sim 45$, or in other words the effective interactions extend to between two and three lattice spacings. Obviously for real physical systems the model of equivalent interactions with cutoff is only a rough approximation to the true situation, but the effective z is a useful indicative phenomenological parameter.

For Xe, the observed effective a_χ corresponds to an effective sc Ising coordination number $z \sim 55$. When data for some other fluids are expressed graphically in terms of $\gamma_{\rm eff}(\tau)$,[8] $\gamma_{\rm eff}$ initially increases slightly with increasing temperature, meaning that a_χ is negative. [The experimental fluid data sets generally extend only over a narrow temperature range above T_c; for small τ, $\gamma_t(t)$ is practically indistinguishable from $\gamma_\tau(\tau)$ and values estimated for a_χ are not sensitive to which scaling expression is used.] Negative a_χ values have been observed in all aqueous electrolyte solutions and also in many nonaqueous

ionic solutions.[42] It has been suggested[8] that as a general rule, simple fluids have positive a_χ and complex fluids negative a_χ. A comparison with Table I and Fig. 3 indicates that for the negative a_χ "complex" systems, the effective coordination number z is 12 or less, so interactions can be considered "short range," while the positive a_χ systems have much higher effective z values and can be classed as having "long-range" interactions.

The effective coordination number is a fundamental parameter for understanding the magnetism of metallic ferromagnets, which can often be considered either from a band or from a local moment perspective. In the case of liquids, it should be possible to make a systematic classification of effective coordination numbers and to link these z values to the interatomic potentials used for calculating structure functions.

V. CONCLUSION

In conclusion, the analysis given above leads to a simple overall physical scenario in which for a family of 3D Ising models, the temperature dependence of the reduced susceptibility over the entire temperature range from T_c right up to infinite temperature is explained using the critical RGT formalism with appropriate Wegner corrections, and without the need to invoke a restricted "critical region" or any form of high-temperature crossover. The approach is conceptually economical and leads to a transparent interpretation of the differences in behavior from model to model and from system to system within a universality class; there is a strong correlation between the coordination number (or, in other words, the "range" of the interactions) and the strength of the nonuniversal amplitude a_χ of the leading confluent Wegner term, which dominates the corrections in all the models we have studied.

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