Critical Properties from Monte Carlo Coarse Graining and Renormalization

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The distribution function $P_L(s)$ of the local order parameter s in finite blocks of size L^d is studied for Ising models for dimensionalities $d=2$, 3, and 4 by Monte Carlo methods. A real-space renormalization group based on phenomenological scaling yields fairly accurate results for rather small L (e.g., the standard exponents β and ν for $d=3$ are found as $2\beta/\nu=1.03\pm0.01$, $1/\nu=1.60\pm0.05$). The method can easily be generalized to arbitrary Hamiltonians, including spin dimensionalities $n>1$.

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Recently numerical real-space renormalization group (RG) methods have yielded accurately the critical behavior of a variety of models.[1-10] Nightingale's[1] RG (based on finite-size scaling[11]), where a fixed point of the scaling relation $\xi_L(K)=b\xi_{L/b}(K')$ for the correlation length $\xi_L(K)$ of an (otherwise infinite) strip of width L at coupling constant K is studied for scale factors $b\to1$, needs transfer matrix methods and thus is restricted to both $d=2$ and models with discrete degrees of freedom (such as Ising and Potts models, etc.). The Monte Carlo renormalization group (MCRG),[4-10] on the other hand, can also be applied to higher d.[8] Apart from the special $d=2$ Heisenberg model,[10] applications to models with continuous degrees of freedom are not yet very successful.[12] Disregarding polymer studies,[6] all real-space RG studies do not exhibit a truly Gaussian fixed point. Thus it is worthwhile to construct still another version of MCRG, which is well suited for studying systems at $d=3$, including continuous degrees of freedom.

In the present work, this problem is treated by a phenomenological RG of the order-parameter distribution function $P_L(s)$ and its moments. As a motivation, we recall the field-theoretic RG approach[13-15] in a form appropriate for a Monte Carlo calculation in real space: Dividing the (Ising) ferromagnet into blocks of size L^d, the spin field representing the magnetization of the blocks $\{s_i\}$ is governed by the probability

$$P_L(\{s_i\})\propto\exp[-\mathcal{H}_{\rm GLW}(\{s_i\})],$$

$$\mathcal{H}_{\rm GLW}(\{s_i\})=\sum_i(r_Ls_i^2+u_Ls_i^4+v_Ls_i^6+\cdots)+\sum_{\langle i,j\rangle}C_L(s_i-s_j)^2+\cdots,$$

with $\langle i,j\rangle$ denoting a summation over nearest-neighbor blocks. One now wishes to study the change of the parameters $\{r_L,u_L,v_L,C_L,\dots\}$ characterizing the Ginzburg-Landau-Wilson Hamiltonian upon changing the length scale, and to study the approach towards the fixed point. Clearly, there would be several useful applications of an explicit realization of such a coarse graining by Monte Carlo method: (i) For a given microscopic Hamiltonian, the set of "initial values" $\{r_L,u_L,v_L,C_L,\dots\}$ of the RG transformation can be identified. We suggest the application of this method to cases where it is uncertain to the vicinity of which fixed point certain Hamiltonians belong. (ii) Using blocks to size $L\approx\xi_\infty(K)$ or larger one gains information on the coarse-grained free-energy functional to be used in studies of nucleation and spinodal decomposition.[16,17] (iii) Critical properties (exponents, critical temperature T_c, etc.) can be found from the behavior near and at the fixed point.

It is only this last application which is presented here. In addition, rather than considering the full distribution $P_L(\{s_i\})$ it is more convenient for numerical work to restrict attention to the reduced distribution $P_L(s)$ of only one block. This function, whose fixed-point behavior is crucial for understanding structural phase transitions,[18] is also well suited for a RG analysis. Rather than fitting parameters r_L, u_L, and v_L to $P_L(s)$, we study the moments $\langle s^k\rangle_L=\int ds\, s^k P_L(s)$, $k=2$, $4,6,\dots$, and the lowest-order cumulants such as $U_L=1-\langle s^4\rangle_L/(3\langle s^2\rangle_L^2)$, $V_L=1-\langle s^4\rangle_L/(2\langle s^2\rangle_L^2)+\langle s^6\rangle_L/(30\langle s^2\rangle_L^3)$. Above T_c, $P_L(s)$ becomes a Gaussian for $L\gg\xi$, and hence $U_L,V_L,\dots$ tend to zero. Below T_c, $P_L(s)$ tends towards two Gaussians centered at $\pm M$, the spontaneous magnetization, and hence $U_L,V_L,\dots$ approach nonzero (but trivial) values ($U_L\to\frac{2}{3}$, etc.). Right at T_c, U_L, $V_L,\dots$ approach nontrivial "fixed-point values" $U^*,V^*,\dots$. We interpret $U^*=V^*=\cdots=0$ as the $T=\infty$ fixed point, $U^*=\frac{2}{3}$ as the $T=0$ fixed point. Thus, studying the ratios $U_{L'}/U_L$, $V_{L'}/V_L$ as functions of T, one finds T_c where the ratios become unity: In contrast to standard Monte Carlo analysis of critical phenomena[19] the estimate of T_c is independent of the exponent estimates.[20]

Extracting exponents is understood by phenomenological scaling, similar to the finite-size RG.[1, 11] Supposing that $P_L(s)$ depends on L, s, and ξ in scaled form, $P_L(s) = L^y \tilde{P}(sL^y, \xi/L)$, where y is an appropriate exponent, and $\tilde{P}(x_1, x_2)$ the associate scaling function, we find $\langle s^k \rangle_L = L^{-ky} f_k(\xi/L)$, where $f_k(x)$ is another scaling function and y is related to the exponents β, ν $[M \propto (1 - T/T_c)^\beta$, $\xi \propto |1 - T/T_c|^{-\nu}]$ as $y = \beta/\nu$. Defining a function W_β as $-W_\beta = \ln[\langle s^2 \rangle_{bL} / \langle s^2 \rangle_L]/\ln b$, we identify β/ν from its fixed-point value, $W_\beta^* = 2\beta/\nu$. The short-range correlations in $\langle s^k \rangle_L$ involve an energylike singularity at T_c, and thus $f_k(x \gg 1) \approx f_k(\infty) + f_k' x^{-(1-\alpha)/\nu} + \cdots$. From this expression one can show that $(\partial U_{bL}/\partial U_L)|_{U^*} = b^{(1-\alpha)/\nu} = b^{d-1/\nu}$, invoking the scaling law $d\nu = 2 - \alpha$.

This approach was applied to Ising lattices with N^d sites and periodic boundary conditions, for $N = 60$ ($d = 2$), $N = 24$ ($d = 3$), and $N = 12$ ($d = 4$). We hence used $L = 2, 3, 4, 5, 6, 10, 12, 15, 20$ ($d = 2$); $L = 2, 3, 4, 6, 8, 12$ ($d = 3$); $L = 2, 3, 4, 6$ ($d = 4$). Clearly, for such small L one expects that (i) $P_L(s)$ does not yet resemble a continuous function, and (ii) corrections to the scaling form of $P_L(s)$ are very important. However, $P_L(s)$ did behave like a continuous function down to $L = 2$ (Fig. 1). Since from *one* Monte Carlo run we obtain $P_L(s)$ for *all* L simultaneously, and each single Monte Carlo step (MCS) contributes to all $P_L(s)$, we achieve reasonable accuracy with moderate effort ($\sim 10^4$ MCS per site). Rather than studying $P_L(s)$ where the block is the subsystem of an infinite system, one can also study the distribution functions $P_L^{(p)}(s)$ and $P_L^{(f)}(s)$ of finite systems of size L^d with periodic (p) or free (f) boundary conditions. While these functions are interesting for understanding metastability,[21] one needs separate runs for each L. As corrections to scaling are more important,[22] we concentrate on subsystem blocks here.

Figure 2 shows the "flow diagram" for U_L. The behavior at $d = 2, 3$ is found as anticipated above. The (universal[22]) numbers $U^* \cong 0.52$ ($d = 2$) and $U^* \cong 0.21$ ($d = 3$) compare reasonably to a calculation[18] using Wilson's approximate recursion relations[13] which yields $U^* \cong 0.58$ ($d = 2$), $U^* \cong 0.22$ ($d = 3$). The results for $d = 4$ suggest $U^* = 0$, i.e., a Gaussian fixed point! The well-defined meaning of Gaussian fixed points in this MCRG is a particular advantage.

The inset of Fig. 1 shows the procedure outlined above for estimating T_c and β/ν: $U_{L'}/U_L$ varies smoothly with T, and estimating T_c presents no difficulty. We get $k_B T_c / J \approx 4.550$ (J is the nearest-neighbor exchange), while the value due to high-temperature series (HTS) is[23] $k_B T_c / J \cong 4.510$. This 1% discrepancy shows that corrections to scaling (important for our small L) affect this (and the exponent) estimate. Assuming corrections of the form

$$\langle s^k \rangle_L |_{T_c} = L^{-k\beta/\nu} f_k(\infty)(1 + f_k^c L^{-x_c} + \cdots),$$

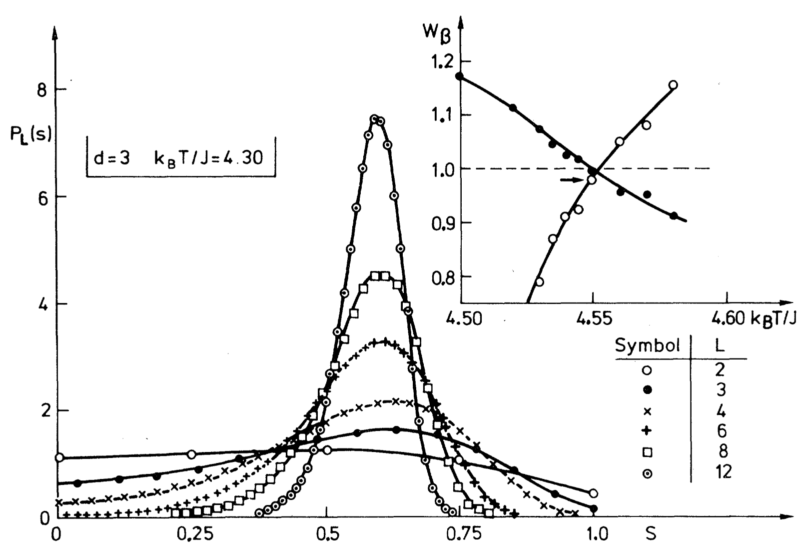

FIG. 1. Block distribution function $P_L(s)$ plotted vs s for various L, for the $d = 3$ Ising model at a temperature 4.66% below T_c. The inset shows W_β (open circles) and $U_{L'} U_L$ for $L' = 6$, $L = 4$; the arrow indicates the estimate for $2\beta/\nu$.

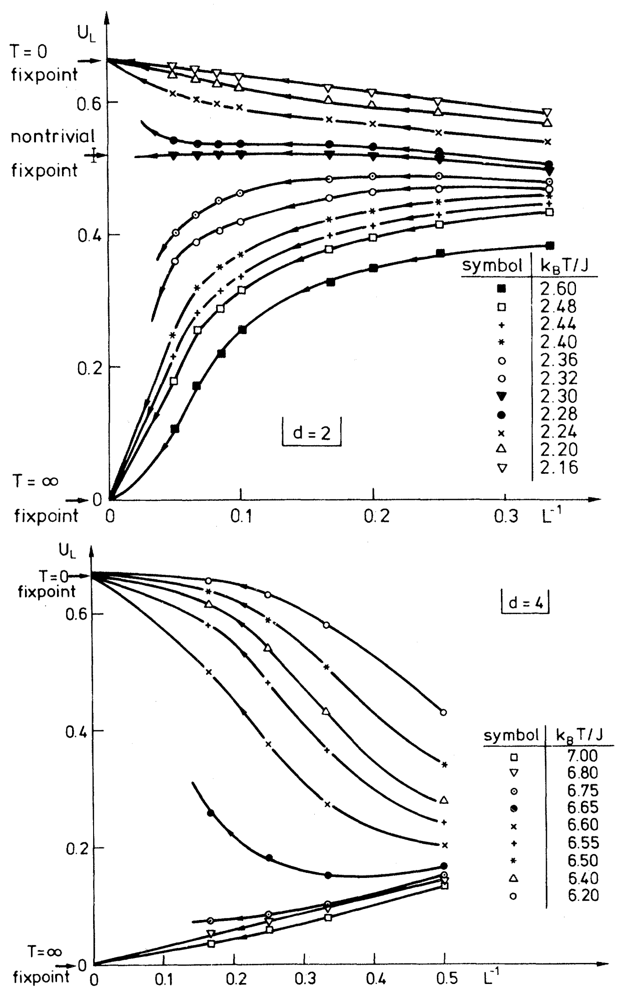

FIG. 2. Cumulant U_L plotted vs L^{-1} for various temperatures and $d = 2$ (upper part) as well as $d = 4$ (lower part. Arrows indicate the fixed points mentioned in the text.

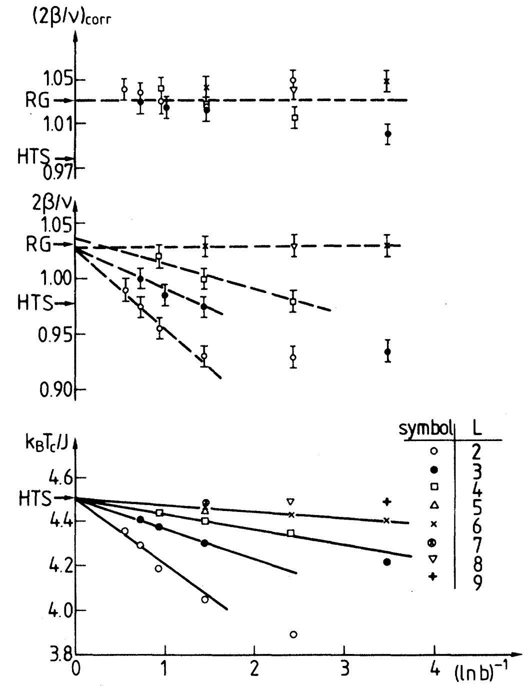

FIG. 3. Critical temperature estimates ($d = 3$) from free blocks plotted vs $(\ln b)^{-1}$ for various L (lower part); estimates for $2\beta/\nu$ for subsystem blocks (middle part); finite-size-corrected exponents, cf. text (upper part). RG (Ref. 15) and HTS estimates (Ref. 23) are indicated by arrows.

the function W_β at T_c becomes

$$W_\beta{}^* = 2\beta/\nu - f_2{}^c L^{-x_c}(1 - b^{-x_c})/\ln b + \cdots .$$

Hence we extrapolate the results as functions of $(\ln b)^{-1}$, Fig. 3: Even for small free blocks, where some estimates for T_c are far off, the data converge to a *unique* limit (the T_c of the HTS), irrespective of L. Free blocks do not yield accurate exponent estimates,[22] but subsystem blocks yield better results: We find $2\beta/\nu = 1.03 \pm 0.01$, in very good agreement with field-theoretic renormalization.[15] Our Hamiltonian is a discrete Ising system, and not a continuum model as in Ref. 15: This is further evidence that the discrepancy with the HTS result[23] $2\beta/\nu \approx 0.98$ is due to too short series[24]; it should not be taken as evidence that discrete Ising systems and continuum field theory belong to different universality classes.

Fitting $W_\beta{}^*$ to the above form, one finds the upper part of Fig. 3. Although there is no longer a systematic dependence on either L or b, the fit parameters $f_2{}^c \approx 0.35$ and $x_c \approx 1.8$ are not very meaningful—presumably several correction terms occur, whose net effect cancels to some extent.

Our $d = 2$ results are similar, though less accurate as W_β is a very steep function of T near T_c (we obtain $2\beta/\nu \approx 0.24 \pm 0.02$). Also the results for $1/\nu$ are somewhat less encouraging, $1/\nu = 1.60 \pm 0.05$ ($d = 3$) and $1/\nu = 0.9 \pm 0.1$ ($d = 2$).[25] However, if we use[22] Monte Carlo data of the same runs in a standard Monte Carlo analysis (fitting straight lines to log-log plots of magnetization, etc.), the results are inconclusive, errors being 15% or larger.

In conclusion, we have demonstrated a new method of analyzing Monte Carlo calculations near critical points, using renormalization-group ideas. Neither *a priori* knowledge of T_c nor the use of particular block sizes or transformations is required. It allows for the occurrence of a Gaussian fixed point (Ising model with $d=4$), and yields accurate exponent estimates for $d=3$. A generalization to continuum spins is straightforward by treating the block variable as a vector $\vec{s}$ and sample $P_L(\vec{s})$. Other interesting applications concern continuum models belonging to the Ising class, such as structural transitions or Lennard-Jones fluids. Finally, $P_L(s)$ can also be used to estimate the susceptibility (from the width of the peak in Fig. 1) and the interface tension [from $P_L(s\approx 0)$].[22]

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[20]For small blocks the fixed points $U_{L'}=U_L=U^*$, $V_{L'}=V_L=V^*$, etc., need not occur at the same T. The difference between these estimates serves as a consistency check. In practice the differences between estimates for T_c drawn from different moments are small compared with the systematic dependence of T_c on L itself.

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[24]This result is substantiated by calculations of further terms of the HTS expansion: see B. G. Nickel, to be published.

[25]Effects due to the finite size of the total lattice $(N)^d$ need to be investigated. E.g., there is a shift of T_c due to the finite size of N (Ref. 11). This is also seen in performing extrapolations for T_c using subsystem blocks (Ref. 22).