Coarse grained free energies with gradient corrections from Monte Carlo simulations in Fourier space

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By performing Wang-Landau simulations in Fourier space, we study coarse grained free energies of generalized lattice spin models. The temperature dependence of the lowest order Landau-Ginzburg free energy expansion coefficients of the s^4 metamodel for phase transitions of the Ising universality class for a given coarse-graining length is calculated for the first time and compared to the standard assumptions made in the literature. In particular, the assumption that the so-called gradient coefficient is constant with temperature is in excellent agreement with the simulations. Our results also indicate that the coarse grained potentials follow finite size scaling. Finally, a coarse grained free energy with a temperature-dependent coarse-graining length equal to the system's correlation length is computed. The resulting potentials are compared to their mean-field counterparts.

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The notion of coarse graining (CG) has proven useful in many different branches of the physical sciences. Usually, what is meant is that a microscopically rapidly oscillating quantity, whose short-range details are irrelevant to the problem under investigation, is replaced by a comparatively slowly varying continuous macroscopic quantity using a smooth spatial averaging procedure defined on a much larger length scale. Examples of such a procedure include the derivation of Maxwell's equation for a macroscopic system or that of the Navier-Stokes equation for hydrodynamic flow.

In statistical mechanics, the behavior of phase transitions on length scales longer than spatial correlations of the microscopic degrees of freedom is frequently described effectively by a smooth order parameter field.[1] In principle, the construction of the associated CG free energies consists of an averaging over the spurious microscopic degrees of freedom, which gives rise to an effective potential with temperature-dependent couplings. Although this averaging is the crucial step in deriving meso- and macrophysics from microscopic Hamiltonians, it is rarely performed explicitly. Instead, one usually resorts to phenomenology augmented by symmetry and universality arguments for the general form of the effective free energy and the behavior of its coefficients. Qualitative and quantitative results of various approximation schemes, such as mean-field theory, provide additional guidance and inspiration. In the context of Wilson and Kogut's momentum shell renormalization,[2] where a similar averaging is performed iteratively near criticality, these assumptions are justified by appealing to the concepts of universality and relevant vs irrelevant couplings. However, CG [in this context, commonly called "Landau-Ginzburg" (LG)] functionals are also often used to describe *noncritical* systems under similar assumptions. A validation of these assumptions is therefore extremely important.

CG densities and the associated free energies are also introduced in a slightly different but intimately related context, namely, the study of metastable states and their decay,[3] where forcing a system to stay homogeneous over regions larger than a certain length scale l to inhibit nucleation of the metastable into the stable phase leads to studying CG partition functions with l chosen to be of the order of the correlation length $\xi(T)$ (Refs. 4–6) as opposed to l fixed.[7]

Early Monte Carlo (MC) simulation attempts to—approximately—determine CG free energies of Ising spin models can be traced back to the early 1980s,[8–10] and research in this direction is still active (see, e.g., Ref. 11 and references therein). However, to our knowledge, coarse grained Landau-Ginzburg free energies including gradient corrections, let alone the full $\boldsymbol{k}$ dispersion, have never been calculated from simulations. Most likely, this is due to the use of real-space algorithms, which we observe to suffer from several serious drawbacks. To start with, there are generally only few possibilities for dividing a finite lattice of manageable size into commensurable subcells, thus putting severe constraints on the choice of possible CG length scales. Moreover, being forced to keep the system homogeneous on the CG level,[14] each total MC move must be constructed from instantaneous coordinated trial moves in all subcells, yielding large accompanying energy changes. Even if parallelization is used for energy computations, such algorithms are thus quite inefficient, as they are troubled by low MC acceptance rates. Also, it is far from clear how to accurately compute gradient corrections from such an approach.

Our strategy is to avoid these difficulties by performing *MC simulations in Fourier space*.[12] Let $s_{\boldsymbol{x}}$ denote a classical "spin" variable in a three-dimensional simple cubic lattice with $N=L^3$ sites $\boldsymbol{x}$, lattice constant $a=1$, and periodic boundary conditions. For L even, the components of the corresponding discrete Brillouin zone $\boldsymbol{k}$ vectors are parametrized by $k_i=2\pi m_i/L$, with integers $m_i=-L/2-1,\ldots,0,\ldots,L/2$. Furthermore, $[\boldsymbol{k}]=[\boldsymbol{k}']$ denotes identity of two general $\boldsymbol{k}$ vectors up to a reciprocal vector. In particular, we write $\boldsymbol{k}^* := [-\boldsymbol{k}]$. Finally, a lattice delta function $\Delta_{\boldsymbol{K}}=\delta_{[\boldsymbol{K}],[\boldsymbol{0}]}$ is defined as a "delta function up to reciprocal vectors." As Ising constraints $s_{\boldsymbol{x}}^2=1$ lead to unmanageable interdependences of the discrete Fourier modes $\tilde{s}(\boldsymbol{k}) := N^{-1/2}\Sigma_{\boldsymbol{x}} s_{\boldsymbol{x}} e^{i\boldsymbol{k}\boldsymbol{x}}$ of a spin configuration $\{s_{\boldsymbol{x}}\}$, we investigate the s^4 model with a Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\sum_{x,y} J(x-y)s_x s_y + \sum_x \left(\frac{\tilde{A}_2}{2}s_x^2 + \frac{1}{4}s_x^4\right) \tag{1}$$

composed of an anharmonic potential with parameter $\tilde{A}_2$ and a short-ranged lattice interaction $J(x-y)$ for real-valued s. In terms of modes, $\beta\mathcal{H}=\beta\mathcal{H}^{(2)}+\beta\mathcal{H}^{(4)}$, where

$$\beta\mathcal{H}^{(2)} := \frac{1}{2}\sum_k [-\tilde{K}(k)+\tilde{A}_2]\tilde{s}(k)\tilde{s}(k^*), \tag{2}$$

$$\beta\mathcal{H}^{(4)} := \frac{\beta}{4N}\sum_{k_1\ldots k_4} \tilde{s}(k_1)\cdots\tilde{s}(k_4)\Delta_{k_1+\cdots+k_4}, \tag{3}$$

with $\tilde{K}(k) := \beta\tilde{J}(k)$ and $\tilde{a}_2 := \beta\tilde{A}_2$. If we want to use $\Re\tilde{s}(k)=\Re\tilde{s}(k^*)$ and $\Im\tilde{s}(k)=-\Im\tilde{s}(k^*)$ as MC variables, we must express the energy in terms of these real degrees of freedom. This is easy for the diagonal quadratic part:

$$\beta\mathcal{H}^{(2)} = \frac{1}{2}\sum_k [-\tilde{K}(k)+\tilde{A}_2]\{[\Re\tilde{s}(k)]^2+[\Im\tilde{s}(k)]^2\}. \tag{4}$$

In contrast, the quartic contribution (3) is complicated by the matching conditions of the four k vectors, making a straightforward calculation of the total energy for a given configuration of modes computationally extremely expensive. However, running any MC-type algorithm based on using the real variables $\Re\tilde{s}(k)$, $\Im\tilde{s}(k)$, only requires the ability to calculate the energy *changes* resulting from shifts $\delta\Re\tilde{s}(k)$, $\delta\Im\tilde{s}(k)$ of these variables, but even this seems difficult. Note, however, that $s_x^4=(s_x^2)^2$. So, in terms of the modes,

$$\widetilde{(s^2)}(k) = \frac{1}{\sqrt{N}}\sum_q \tilde{s}(q)\tilde{s}([k+q^*]) \tag{5}$$

of the *squared* spins s_x^2, $\beta\mathcal{H}^{(4)}$ is "diagonal:"

$$\beta\mathcal{H}^{(4)} = \frac{\beta}{4}\sum_k \widetilde{(s^2)}(k)\widetilde{(s^2)}(k^*). \tag{6}$$

A calculation of $\beta\mathcal{H}^{(4)}$ according to this equation requires not only to store the complex numbers $\tilde{s}(k)$ but also to keep track of the complex modes $\widetilde{(s^2)}(k)$. However, this bookkeeping effort is rewarded, as it allows us to determine both the resulting shifts $\delta\widetilde{(s^2)}(k)$ and the resulting change of total energy from a set of formulas of manageable complexity and corresponding algorithm with reasonable computational costs.

To generate observables related to spatial correlations, the system is extended to include a coupling of spins to an external inhomogeneous field h_x, usually taken to be bilinear, i.e., of the form $\Sigma_x h_x s_x=\Sigma_k\tilde{h}(k)\tilde{s}(k^*)$. In particular, to study *long-range* correlations near phase transitions, small fields h_x containing *only long wavelength* variations, i.e., only modes with minimal wavelength l, need to be considered. In other words, we assume a cutoff $\Lambda=2\pi l/L$ such that $\tilde{h}(k)=0$ for $|k_i|>\Lambda$. This also suggests to split $s_x\equiv\eta_x+\varphi_x$ into "slow" and "fast" modes $\eta_x := \frac{1}{\sqrt{N}}\Sigma_{|k_i|\leq\Lambda}\tilde{s}(k)e^{ikx}$ and $\varphi_x := s_x-\eta_x$, respectively, such that only the slow ones couple to h_x. The fast modes $\tilde{s}(k)$ can be integrated out of the canonical partition function $Z[h]=\int\mathcal{D}s e^{-\beta H[s]+\Sigma_x h_x s_x}$ such that remaining effective Hamiltonian $H^{(L,l)}[\eta]$ for the slow modes, defined by

$$Z[h] \equiv e^{-\beta N u_0}\int \mathcal{D}\eta e^{-\beta H^{(L,l)}[\eta]+\Sigma_{|k_i|\leq\Lambda}\tilde{h}(k)\tilde{\eta}(k^*)}, \tag{7}$$

is *independent of* h_x. However, $H^{(L,l)}[\eta]$ is our *coarse grained* Hamiltonian of the original system at scale l. By symmetry arguments,[2] it must be of the general form

$$\begin{aligned}\beta H^{(L,l)}[\eta] = {} & \frac{1}{2}\sum_k u_2^{(L,l)}(k)\tilde{\eta}(k)\tilde{\eta}(k^*) + \frac{1}{4N}\sum_{k_1,\ldots,k_4} u_4^{(L,l)} \\ & \times(k_1,\ldots,k_4)\tilde{\eta}(k_1)\cdots\tilde{\eta}(k_4)\Delta_{\Sigma_{i=1}^4 k_i} \\ & + \frac{1}{6N^2}\sum_{k_1,\ldots,k_6} u_6^{(L,l)} \\ & \times(k_1,\ldots,k_6)\tilde{\eta}(k_1)\cdots\tilde{\eta}(k_6)\Delta_{\Sigma_{i=1}^6 k_i}+\cdots,\end{aligned} \tag{8}$$

where the coefficients $u_i^{(L,l)}$ can be assumed to be symmetric in their arguments. Let us first focus on the coefficient for the quadratic term, $u_2^{(L,l)}(k)=u_2(0)+\beta D(k)$. For the particular η configuration

$$\tilde{\eta}_Q(k) \equiv \Re\tilde{\eta}_Q(k) \equiv \begin{cases} r\in\mathbb{R}, & k=Q,Q^* \\ 0 & \text{else}, \end{cases} \tag{9}$$

we have

$$\beta H^{(L,l)}[\eta_Q] = \begin{cases} u_2^{(L,l)}(0)r^2/2+O(r^4), & Q=0 \\ u_2^{(L,l)}(Q)r^2+O(r^4), & Q\neq 0. \end{cases} \tag{10}$$

Constraining all other slow s modes with $k\neq Q$, as well as $\Im\tilde{\eta}_Q(k)$ to be zero, $P_Q(r) := e^{-\beta H^{(L,l)}[\eta_Q]}$ is proportional to the probability distribution for the remaining real amplitude r of $\tilde{\eta}_Q(k)$ in the "bath" of all fast modes $\tilde{\varphi}(k)$. In MC sampling, the real and imaginary parts of these fast modes serve as the degrees of freedom. In performing a MC move, one of these real numbers is randomly chosen and shifted by an amount drawn at random from a fixed interval. Since the same "phase space" volume is available to forward and backward moves and the resulting energy change is fed into the Metropolis rule, detailed balance is thus guaranteed. As straightforward MC is not well suited to explore potential barrier structures, we calculate $P_Q(r)$ in a Wang-Landau simulation.[13–15] Collecting parameters of parabolic fits to $-\ln P_{Q_i}(r)$ around $r=0$ for, e.g., vectors $Q_i=(2\pi m_i/L,0,0)$, $m_i=0,\ldots,l$, we obtain the values $u_2(Q_i)$ [and thus $u_2(0)$ and the dispersion $D(Q_i)$]. In addition, we can also determine the values $u_4(0),u_6(0),\ldots$ from fitting the negative logarithm $-\ln P_0(r)$ of the analogous zero mode probability distribution $P_0(r)$ to a polynomial of sufficiently high order. This strategy allows us to determine all the coefficients defining a "classical" LG Hamiltonian.

To test our algorithm, we performed simulations of the s^4 model with nearest-neighbor interaction on $3d$ lattices of size $L=12$ and CG scale $0\leq l\leq 5$, parametrized by a coupling

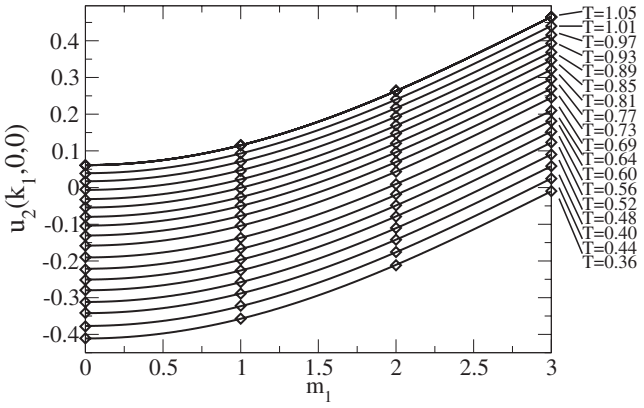

FIG. 1. Plot of $u_2^{(12,4)}(k,0,0)/\beta$ for various temperatures. Lines are fits by $u^{(12,4)}(k_1,0,0)/\beta = u_2^{(12,4)}(\mathbf{0})/\beta + 4D_0 \sin^2(k_1/2)$.

constant $J \equiv 2C$ and $\tilde{A}_2 := -1 + 12C$, for $C = 0.1$. For various temperatures, sets of curvatures were calculated from fitting the dispersions $-\ln P_{(k_i,0,0)}(r)$ around $r=0$. These were then in turn fitted to the rather rigid ansatz $\beta D(\boldsymbol{k}) = 4\beta D_0 \Sigma_{i=1}^{3} \sin^2(k_i/2)$ suggested by the Fourier transform of the "bare" nearest-neighbor interaction. The corresponding fits were found to be excellent (see Fig. 1). Moreover, the only free parameter D_0 remains quite close to the bare value $D_0 \equiv J = 2C$ obtained by neglecting any thermal or anharmonic effects. In particular, the whole dispersion $D(\boldsymbol{k})$ is practically constant with temperature. This observation—for the first time—directly supports the corresponding assumption usually made in the LG theory. Results for $(L,l) = (12,4)$ are displayed in Fig. 2.

The function $H^{(L,l)}(\boldsymbol{\eta_0})$ represents the homogeneous (Landau) contribution to the CG effective Hamiltonian $H^{(L,l)}[\boldsymbol{\eta}]$. Figure 3 shows the results for the parameters $A_{2k}^{(L,l)}$, $k = 1,2,3$ obtained for $H^{(L,l)}[\boldsymbol{\eta_0}]/L^3$ from a fit to a polynomial $F^{(L,l)}(m) = N\Sigma_{k \leqslant 5} A_{2k}^{(L,l)}/(2k) m^{2k}$ where we changed the argument of $H^{(L,l)}$ from $\boldsymbol{\eta_0}$ to the average "magnetization" per site $m := N^{-1}\Sigma_{\boldsymbol{x}} s_{\boldsymbol{x}} = N^{-1/2}\tilde{s}(\mathbf{0}) = N^{-1/2}\tilde{\eta}(\mathbf{0})$. As expected from the general fluctuation theory, the temperature $T_c^{(L,l)}$,

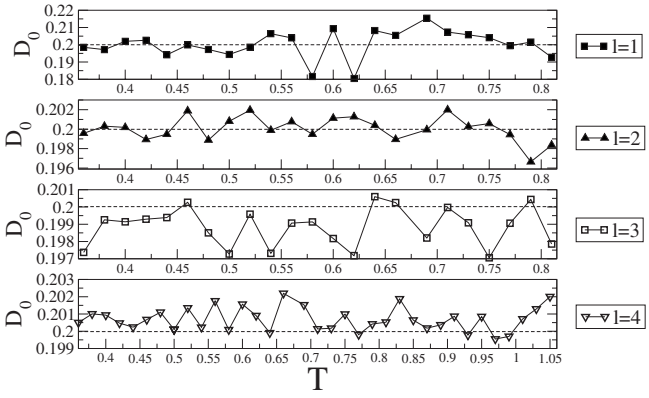

FIG. 2. T dependence of fit parameter D_0 for $L=12$ and $l = 1,\ldots,4$ [the fluctuations in the obtained values for D_0 are observed to be relatively large for $l=1$ for trivial reasons: in this case, only two points $(m_i = 0,1)$ are available to the fits].

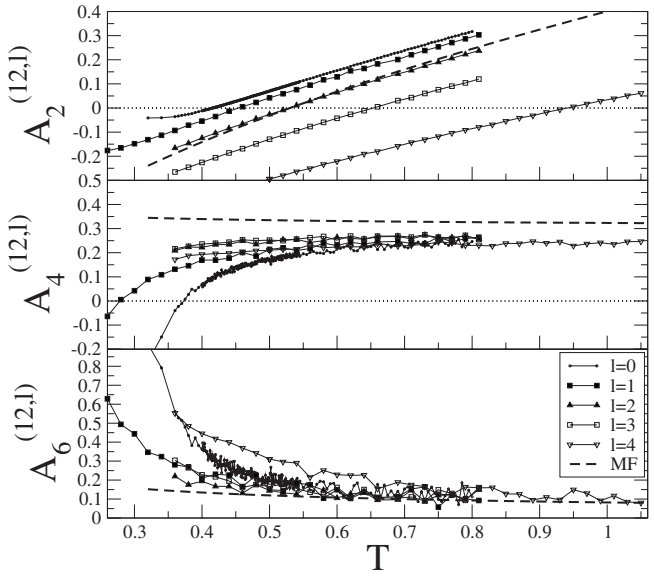

FIG. 3. T dependence of fit parameter $A_{2k}^{(12,l)}$ for $k = 1,2,3$ and $l = 0,\ldots,4$. Broken lines indicate mean-field results.

which we define as the temperature at which the potential shape changes from single to double well, increases with increasing l. For $L=12$ and $l = 0,\ldots,4$, a tenth order polynomial fit yields the values $T_c^{(12,l)} = 0.4152,\ 0.4557,\ 0.5272,\ 0.6525,\ 0.9380$. For $l > L/2$, $H^{(L,l)}$ trivially collapses to the original microscopic Hamiltonian $\mathcal{H}$ [implying $T_c^{(L,l)} = \infty$], while $T_c^{(L,0)} \equiv T_c^{(L)}$ is just the finite size transition temperature of the unconstrained model. For $l=0$, we observe an upward bend in the $A_2^{(L,l)}$ coefficient below T_c, indicating phase separation.[14] Comparison to the cases $l>0$ shows that our CG constraint quite efficiently inhibits this phase separation: neither the notorious downward "kinks" found, e.g., in Refs. 16 and 17, nor the pronounced upward bend in $A_2^{(L,l>0)}$ is observed within the simulated temperature range (except maybe for $l=1$). Near $T_c(L,l)$, the coefficients $A_2^{(L,l)}$ are roughly linear in $T - T_c^{(L,l)}$, their slope comparable to the mean-field theory result. Replacing $H^{(L,l)}$ by the dispersion term $\beta D(\boldsymbol{k})$, combined with a pure 2-4 "Landau" potential with coefficients calculated from a brute force fit to $H^{(L,l)}(\tilde{\boldsymbol{\eta}}_{\boldsymbol{0}})$, it was possible to reconstruct the full partition function from summing over the remaining modes $\tilde{\eta}(\boldsymbol{k})$ with satisfying accuracy.

A standard finite size scaling (FSS) analysis of the Binder cumulants $B_4(T) = 1 - \langle m^4 \rangle / 3\langle m^2 \rangle^2$ for lattices of sizes $L = 6-14$ yields a bulk critical temperature $T_c = 0.405\,87$ some 2.2% lower than $T_c^{(12,0)}$. From the slopes of the Binder cumulant at T_c, we moreover estimate the exponent $\nu \approx 0.62$ in nice agreement with Ising universality. As to the FSS scaling properties of the potentials $H^{(L,l)}$ (see Ref. 18), FSS can only be expected to hold for those families of potentials $H^{(L,l)}$ resulting from summing over the same fractional Brillouin zone volume. This gives rise to a class arrangement according to a common label $\sigma(L,l) := L/(2l+1)$. The lowest *triple* of such systems with manageable sizes L is $\{(6,\ 1),\ (10,\ 2),\ (14,\ 3)\}$ for which $\sigma = 2$. We report that the corresponding Binder cumulants again nicely intersect at a common "bulk

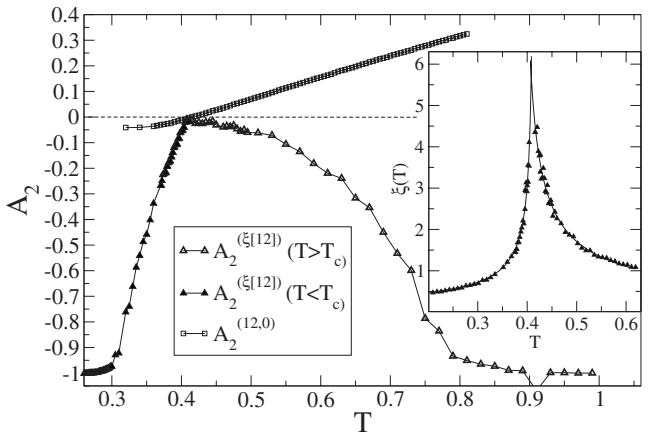

FIG. 4. $A_2^{(\xi[12])}$ for $T<T_c^{(12)}$ (full triangles) and $T>T_c^{(12)}$ (open triangles) vs $A_2^{(12,0)}$ (open boxes). Inset: Fit of correlation length to $\xi(T)\sim(T-T_c)^{0.62}$.

transition temperature" $T_c^{(2)}\approx 0.5782$. This indicates that the FSS hypothesis holds for the above family of potentials $H^{(L,l)}$.

To calculate CG potentials with a temperature-dependent cutoff $\pi/\xi(T)$, we first performed MC simulations of the correlation function $\tilde{G}_c(\boldsymbol{k}) := \langle \tilde{s}(\boldsymbol{k})\tilde{s}(\boldsymbol{k}^*)\rangle - \tilde{s}^2(\boldsymbol{0})$, from which ξ was calculated utilizing[19] $\xi^2(T) = -\partial \ln \tilde{G}_c(\boldsymbol{k})/\partial k^2|_{\boldsymbol{k}=\boldsymbol{0}}$. The resulting behavior of $\xi(T)$ conforms nicely to $\nu=0.62$, as can be seen from a fit displayed as an inset in Fig. 4. As expected, the behavior of the resulting potential coefficients, denoted as $A_{2k}^{(\xi[L])}$, is qualitatively different from those obtained for fixed cubic cutoff. In particular, while $A_2^{(\xi[L])}$ also approaches zero at $T_c^{(12)}$ from below, its slope is markedly steeper than $A_2^{(12)}$ [see Fig. 4 for $L=12$; for illustration, the figure also includes a plot of the formally definable branch $A_2^{(\xi[12])}$ for $T>T_c^{(12)}$, which, however, seems to have no direct physical interpretation]. This behavior results from an imposed and controlled homogeneity constraint and is similar to the "kinks" found in, e.g., Refs. 16 and 17. There, phase separation below T_c was most likely prevented by the finite MC sampling time. In addition, note that for extremely high or low temperatures $\xi\to 0$, so no more modes are left to sum over, implying that the potential becomes trivially identical to the microscopic Hamiltonian. This is illustrated by the tendency of $A_2^{(\xi[L])}$ to saturate at the value -1 for these limits (see Fig. 4).

Using fast Fourier transformation, combined with energy calculations in real space, a similar coarse-graining procedure could be applied to considerably more general lattice and off-lattice systems. Moreover, our Fourier algorithm is tailor made to study the compressible ϕ^4 model with elastic anisotropy. This model is extremely hard to tackle using "conventional" MC simulations,[20] because the corresponding effective Hamiltonians can be written in a manageable way only in terms of Fourier modes.[21]

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[1] K. Binder, in *Materials Science and Technology*, edited by P. Haasen (VCH, Weinheim, 1991), Vol. 5, p. 143.
[2] K. G. Wilson and J. Kogut, Phys. Rep. **12C**, 75 (1974).
[3] J. S. Langer, Physica (Amsterdam) **73**, 61 (1974).
[4] J. S. Langer, M. Bar-on, and H. D. Miller, Phys. Rev. A **11**, 1417 (1975).
[5] K. Kawasaki, T. Imeda, and J. D. Gunton, in *Perspectives in Statistical Physics*, edited by H. J. Raveché (North-Holland, Amsterdam, 1981).
[6] K. Binder, Rep. Prog. Phys. **50**, 783 (1987).
[7] N. G. van Kampen, Phys. Rev. **135**, A362 (1964).
[8] K. Binder, Phys. Rev. Lett. **47**, 693 (1981).
[9] H. Furukawa and K. Binder, Phys. Rev. A **26**, 556 (1982).
[10] K. Kaski, K. Binder, and J. D. Gunton, J. Phys. A **16**, L623 (1983).
[11] M. E. Gracheva, J. M. Rickman, and J. D. Gunton, J. Chem. Phys. **113**, 3525 (2000).
[12] R. H. Swendsen, Phys. Rev. Lett. **47**, 1159 (1981).
[13] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
[14] A. Tröster, C. Dellago, and W. Schranz, Phys. Rev. B **72**, 094103 (2005).
[15] F. Calvo, Mol. Phys. **100**, 3421 (2002).
[16] G. H. F. van Raaij, K. J. H. van Bemmel, and T. Janssen, Phys. Rev. B **62**, 3751 (2000).
[17] T. Radescu, I. Etxebarria, and J. M. Perez-Mato, J. Phys.: Condens. Matter **7**, 585 (1995).
[18] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981).
[19] D. Amit and V. Martin-Mayor, *Field Theory, the Renormalization Group and Critical Phenomena*, 3rd ed. (World Scientific, Singapore, 2005).
[20] X. Zhu, F. Tavazza, D. Landau, and B. Bunwev, Phys. Rev. B **72**, 104102 (2005).
[21] D. J. Bergman and B. I. Halperin, Phys. Rev. B **13**, 2145 (1976), Formula (5.2).