Renormalization groups for two- and three-dimensional kinetic Ising models

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We present a renormalization group for kinetic Ising models. Recursion relations for flip rates are established through double series in powers of the inverse temperature and a self-consistently determined time-scale ratio. A static transformation is obtained as a subset of recursion relations in which only the inverse temperature appears as expansion parameter. Our best second-order value for $d=2$ is $z=2.2$ (with an uncertainty of roughly 10%), while for the simple cubic lattice in $d=3$ we find $z=1.98$ if T_c is adjusted to the known numerical value.

Glauber's kinetic Ising models,[1] defined by flip rates for Ising spins on lattice sites, enjoy an increasing importance for computer simulations of critical phenomena. Analytic treatments of their critical behavior with the help of the real-space renormalization group (RSRG) have also been attempted. However, relative to its impressive success in the determination of static critical exponents,[2] the RSRG has yielded results of rather limited reliability for the dynamical exponent z.[3]

The RSRG transformation for kinetic Ising models relates the flip rates for site spins ($\sigma_i=\pm1$) to flip rates for "cell" spins ($\mu_\nu=\pm1$) which are associated with cells of lattice sites. The corresponding recursion relations must usually be constructed perturbatively, the intercell coupling serving as an expansion parameter. Since intracell bonds are not distinguished physically from intercell bonds, however, such perturbation expansions are nonsystematic unless the intracell interactions are treated perturbatively as well.

The distinction between systematic high-temperature series[4] and usual cumulant expansions[2] is of little importance for the static RSRG. In the dynamic case, on the other hand, nonsystematic expansions in terms of intercell bonds have been shown to yield, of necessity, fewer recursion relations than are needed to construct unique fixed-point flip rates; they therefore do not allow the calculation of the dynamical exponent z unless *ad hoc* assumptions are introduced.[5]

We shall now present a systematic implementation of the dynamic RSRG. We start by representing the flip rates of spins by high-temperature series, neglecting third- and higher-order terms. We illustrate the further procedure for a triangular lattice in $d=2$. Groups of three lattice sites which are all nearest neighbors to one another are taken as cells. The cells form a triangular lattice, too; the ratio of the two lattice constants being $b=\sqrt{3}$.

Intending to find the most general flip rates possible in second order we recall that the corresponding static transformation[4] involves pair interactions between first ($1N$), second ($2N$), and third ($3N$) neighbors; the dimensionless $1N$ bond strength K_1 is of first order in $1/T$, while the $2N$ and $3N$ couplings, K_2 and K_3, are of second order.[4] We must therefore expect the order of any term in the flip rates to be equal to (or larger than) the minimum number of $1N$ bonds necessary to connect all spins involved. According to such a rule, not only single spin flips (SSF) but also double (DSF) and triple (TSF) spin flips can occur in second order.

The probability $P(\sigma,t)$ of finding a certain configuration of site spins obeys a master equation of the form $\dot{P}=LP$. The generator of infinitesimal time translations L can most conveniently be expressed with the help of the operator A_i which antisymmetrizes functions of the spin on the ith lattice site σ_i as

$$A_i f(\sigma_i)=\tfrac{1}{2}[f(\sigma_i)-f(-\sigma_i)] \ .$$

The rule described above then yields an ansatz for L involving 17 parameters. Three of these are the bond strengths K_i already mentioned; their presence manifests detailed balance and thus $Le^{-H}=0$, with

$$H=-\left(K_1\sum_{ij}^{1N}+K_2\sum_{ij}^{2N}+K_3\sum_{ij}^{3N}\right)\sigma_i\sigma_j+\text{const} \ ,$$

to within corrections of order $1/T^3$. Another parameter Γ sets the overall time scale for all flip processes; the remaining 13 parameters describe the detailed structure of TSF rates (χ_1,χ_2,χ_3), DSF rates ($\psi_0,\psi_1,\ldots\psi_6$), and SSF rates ($\phi_1,\phi_2,\phi_3$). The generator in question reads

$$\Gamma^{-1}L=-(1+3K_1^2)\sum_i A_i-\psi_0\sum_{ij}^{1N}A_iA_j+\left(v_1\sum_{ij}^{1N}+v_2\sum_{ij}^{2N}+v_3\sum_{ij}^{3N}\right)A_i\sigma_i\sigma_j-\left(\phi_1\sum_{i<j<k}+\phi_2\sum_{j\frown i\frown k}+\phi_3\sum_{j\frown i-k}\right)A_i\sigma_j\sigma_k$$
$$-\left(\psi_1\sum_{ij}^{1N}+\psi_2\sum_{ij}^{2N}+\psi_3\sum_{ij}^{3N}\right)A_iA_j\sigma_i\sigma_j-\left(\psi_4\sum_{i<j<k}+\psi_5\sum_{j\frown i\frown k}+\psi_6\sum_{j\frown i-k}\right)A_iA_j\sigma_j\sigma_k-\left(\chi_1\sum_{i<j<k}+\chi_2\sum_{j\frown i\frown k}+\chi_3\sum_{j\frown i-k}\right)A_iA_jA_k\sigma_j\sigma_k, \quad (1)$$

with the abbreviations $v_1 = K_1 + \psi_1/2 - \psi_1 K_1$, $v_2 = K_2 + \psi_2/2 - \psi_1 K_1$, $v_3 = K_3 + \psi_3/2 - \psi_1 K_1/2$.

The rule used to find L requires all of the 17 parameters except Γ, K_1, ψ_0, and ψ_1 to be of at least second order; the RSRG to be discussed now gives rise to those other 13 parameters as well as to ψ_0 in second order, while ψ_1, together with K_1, appears in first order; the time scale factor Γ must, of course, be of zeroth order.

We now consider the conditional probability $P(\sigma,t|\sigma')$, i.e., the matrix representative of the operator e^{Lt}. With it we associate a conditional probability $\tilde{P}(\mu,t|\mu')$ for cell spins, with the help of suitable rectangular matrices $R(\mu,\sigma)$ and $\hat{R}(\sigma,\mu)$, as the product[5,6]

$$\tilde{P}(\mu,t|\mu') = R(\mu,\bar{\sigma})P(\bar{\sigma},t|\bar{\sigma}')\hat{R}(\bar{\sigma}',\mu') \quad , \quad (2)$$

where barred variables are to be summed over.

The definition (2) implies, for $t=0$, the identity $R\hat{R} = 1_{\mu\mu'}$. For $t \to \infty$, on the other hand, when $\tilde{P}$ and P go over into the static distributions $e^{-H'(\mu)}$ and $e^{-H(\sigma)}$, respectively, we conclude that (i) $\hat{R}(\bar{\sigma},\mu) = 1$ and (ii) R is the matrix defining the static RSRG.

Since R attaches an Ising spin μ_ν to the νth cell in which there are three site spins $\sigma_{\nu 1}$, $\sigma_{\nu 2}$, and $\sigma_{\nu 3}$, we may specify R as a direct product of matrices R_ν, one for each cell. For the free energy of the site spins to be equal to that of the cell spins we must impose $R_\nu(\bar{\mu}_\nu, \sigma_{\nu 1}, \sigma_{\nu 2}, \sigma_{\nu 3}) = 1$. Symmetry considerations then dictate

$$R_\nu = \tfrac{1}{2}[1 + \mu_\nu \phi(\sigma_{\nu 1}, \sigma_{\nu 2}, \sigma_{\nu 3})] \quad , \quad (3)$$

where ϕ is an arbitrary linear combination of the sum $s_\nu = (\sigma_{\nu 1} + \sigma_{\nu 2} + \sigma_{\nu 3})\sqrt{24}$ and the product $t_\nu = \sigma_{\nu 1}\sigma_{\nu 2}\sigma_{\nu 3}/\sqrt{8}$. There are thus two free parameters in R, one of which can be fixed by the following dynamical argument.

When going over from site spins to cell spins as in (2), we change the unit of length by a factor $b = \sqrt{3}$. At criticality, however, the lifetime of order-parameter fluctuations increases with their wavelength. For the transformation (2) to be physically sensible the cell spin μ_ν must be associated with the slowest one among the four linearly independent odd-under-spin-reversal functions we can form with $\sigma_{\nu 1}$, $\sigma_{\nu 2}$, and $\sigma_{\nu 3}$. Surely, among those four functions, we must expect one of the two which are symmetric under site permutations within the cell to be slower than the other two, the latter ones living on a shorter length scale. In order to find the most long-lived function of the form described we should, in principle, diagonalize the generator L. It is more in the spirit of the RSRG, however, to base the distinction between slow and fast on the part of L which describes the dynamics within the νth cell L_ν. The diagonalization of L_ν is easily achieved and yields a slowest left-hand eigenfunction of the expected form,

$$\phi = (s_\nu + f t_\nu)p \quad , \quad (4)$$

with arbitrary p and a uniquely determined coefficient f which turns out to be of order $1/T^2$. There is thus one free parameter left in R.

Due to the fact that the generator L has unique stationary right- and left-hand eigenfunctions (e^{-H} and 1, respectively) the matrix $\hat{R}(\sigma,\mu)$ need not be specified. Any choice consistent with the restrictions mentioned yields the same RSRG transformation. A choice which simplifies all calculations is a product $\hat{R} = \prod_\nu \hat{R}_\nu$ with

$$\hat{R}_\nu(\sigma,\mu) = \tilde{\psi}(\sigma_{\nu 1}, \sigma_{\nu 2}, \sigma_{\nu 3})/\sqrt{8} + \mu_\nu \tilde{\phi}(\sigma_{\nu 1}, \sigma_{\nu 2}, \sigma_{\nu 3})/p \quad ,$$

where $\tilde{\psi}$ and $\tilde{\phi}$ are two right-hand eigenfunctions of the intracell generator L_ν, $\tilde{\psi}$ is the stationary eigenfunction, and $\tilde{\phi}$ pertains to the eigenvalue to which ϕ is the left-hand eigenfunction.

Since we want to establish the RSRG as a set of recursion formulas for the 17 parameters given in (1), we proceed from the conditions probability $\tilde{P}(\mu,t|\mu')$ to its generator of infinitesimal time translations:

$$l(t,\mu,\mu') = \dot{\tilde{P}}(\mu,t|\bar{\mu})\tilde{P}^{-1}(\bar{\mu},t|\mu') = (RLe^{Lt}\hat{R})_{\mu\bar{\mu}}[(Re^{Lt}\hat{R})^{-1}]_{\bar{\mu}\mu'} \quad . \quad (5)$$

This generator is a time-dependent matrix.

In expressing the generator $l(t)$ in terms of the original one L we intend to perform an adiabatic elimination.[7] The site-spin problem contains "slow" variables (one per cell, ϕ) and "fast" ones (six per cell); the slow ones are associated with the cell spins and the fast ones are to be eliminated. The time dependence in $l(t)$ is a fast one, characterized by the six largest eigenvalues of the intracell dynamics. After the decay of such fast transients the generator becomes a time-independent matrix $l(\infty,\mu,\mu')$. With the construction of $l(\infty,\mu,\mu')$ the intended adiabatic elimination of the fast variables is achieved. By using the matrix representations $\frac{1}{2}(1+\mu_\nu\mu_\nu')$, $\frac{1}{2}\mu_\nu\mu_\nu'$, $\frac{1}{2}\mu_\nu$, and $\frac{1}{2}(\mu_\nu+\mu_\nu')$ for the operators 1_ν, A_ν, $A_\nu\mu_\nu$, and μ_ν, respectively, the matrix $l(\infty,\mu,\mu')$ may be replaced by an operator identical in structure to L as given by (1). In order to complete the definition of the dynamical RSRG we introduce, as usual, a time dilation factor $b^z = 3^{z/2}$ and write

$$L' = b^z \lim_{t\to\infty} (RLe^{Lt}\hat{R})(Re^{Lt}\hat{R})^{-1} \quad , \quad (6)$$

where the right-hand side is to be understood in the operator sense just explained.

For the explicit evaluation of the transformation (6), we must expand in powers of $1/T$. However, the

infinite temperature version of L, $-\Gamma\sum_i A_i$, has intracell pieces with eigenvalues 0, $-\Gamma$, -2Γ, and -3Γ, the second and third of which are triply degenerate. A naive perturbation expansion of the right-hand side of (6) in powers of $L+\Gamma\sum_i A_i$ is thus bound to produce resonance divergencies.[8] Clearly, such degeneracies must be lifted by diagonalizing a larger part of L, to be called $L^{(0)}$, before we can start expanding in $L-L^{(0)}$. In consistency with our choice for the transformation matrix $R(\mu,\sigma)$, we take $L^{(0)}=\sum L_\nu$, i.e., diagonalize the full intracell dynamics and expand in powers of the intercell part of L, keeping linear and quadratic terms.

Necessary as the partial diagonalization may be, it still tends to yield slightly nonsystematic recursion relations since it distinguishes intracell from intercell bonds. Therefore, in order to deviate as little as possible from a strict $1/T$ expansion, we break up all resulting expressions, with one exception, in their high-temperature series, again dropping all third- and higher-order terms. The exception mentioned concerns terms which would produce resonance divergencies; these terms have in their denominators differences of eigenvalues of L_ν.

It would not even make much sense to keep the terms with dangerous denominators in the form produced by the formal expansion in $L-L^{(0)}$. The adiabatic elimination inherent in (6) is sensible only inasmuch as the eigenvalue pertaining to the slow eigenfunction ϕ of L_ν has small ratios with the six nonzero eigenvalues. We therefore use that ratio as a second expansion parameter, treating it, in counting orders, like $1/T$.

Having laid out our strategy we may leave the detailed calculation, which is lacking neither charm nor algebraic complexity, to a separate paper and turn to the results.

A most satisfactory feature of our RSRG is the strict separation of statics and dynamics. The 17 recursion relations include a closed subset for the bond strengths K_i:

$$\begin{aligned} K_1' &= \frac{p^2}{8}\left(\tfrac{2}{3}K_1+K_2+\tfrac{2}{3}K_3+4K_1^2\right)-\frac{p^4}{72}K_1^2 \ , \\ K_2' &= \frac{p^2}{24}\left(K_3+K_1^2\right)-\frac{p^4}{72}K_1^2 \ , \\ K_3' &= -\frac{p^4}{144}K_1^2 \ . \end{aligned} \tag{7}$$

These equations contain no terms with dangerous denominators. They could have been obtained by using (3) and (4), with $f=O(1/T^2)$, in the static RSRG of Betts *et al.*[4] Since the free parameter p appears in the static RSRG it can be fixed by adjusting the critical temperature to the exact value. This procedure yields a correlation length exponent $\nu=0.87$, a result 13% off the exact one, $\nu=1$.

An alternative way of fixing p which does not involve information alien to the RSRG is the following. Our transformation can be written either as a set of recursion relations for the 17 parameters K_i, ϕ_i, ψ_i, and χ_i, or as a set in which the equations for the static parameters K_i are replaced by those for auxiliary quantities, $v_i-\psi_i/2$. The two versions of our transformation are, of course, equivalent to within corrections of $O(1/T^3)$. They can, however, yield different numerical results since the two sets of parameters are related nonlinearly. Since the fixed-point value of v_1 turns out to react sensitively to such changes of formulation it is natural to fix p by the requirement that both formulations yield the same v_1^*. This choice of p gives a T_c off the exact value by 2% and a critical exponent ν differing from the one found by adjusting T_c by less than 1%.

In order to determine the dynamical exponent z we do not need all 17 recursion relations. In fact, there is, beyond (7), a larger closed subset of seven relations involving the K_i, the auxiliary quantities v_i, and the time-scale parameter Γ. The four remaining equations contain the "slow" eigenvalue of L_ν, $\Gamma\gamma_1=\Gamma(1-2v_1+3K_1^2)$, and one "fast" one, $\Gamma\gamma_2=\Gamma(1+v_1+3K_1^2)$, and read

$$\begin{aligned} b^{-z}\Gamma'(1+3K_1'^2) &= \Gamma\gamma_1-\tfrac{10}{3}\Gamma v_1^2/\gamma_2 \ , \\ b^{-z}\Gamma' v_1' &= \Gamma\left(\tfrac{2}{3}v_1+v_2+\tfrac{2}{3}v_3\right)+\tfrac{4}{9}\Gamma v_1^2/\gamma_2 \ , \\ b^{-z}\Gamma' v_2' &= \tfrac{1}{3}\Gamma v_3-\tfrac{5}{9}\Gamma v_1^2/\gamma_2 \ , \\ b^{-z}\Gamma' v_3' &= -\tfrac{4}{9}\Gamma v_1^2/\gamma_2 \ . \end{aligned} \tag{8}$$

A pocket calculator can be used to locate the fixed-point values K_i^* and v_i^* and then to determine, from the first of Eqs. (8), the dynamical exponent. The result is $z=2.27$ if p is chosen through the self-consistency argument described above; if p if fixed so as to give the right T_c the same value for z results, to within less than 1%.

In extending our method to other lattices and to three dimensions we should expect the results to be less trustworthy the larger the two expansion parameters are, $1/T$ (in practice, v_1^* turns out to be a convenient measure for $1/T$) and the time-scale ratio for slow and fast intracell variables. We have done, with this thought in mind, some explorations for the planar square lattice and the simple cubic lattice in $d=3$. We are led to believe that two-step transformations are most promising.

For the planar square lattice we first group two neighboring sites to a cell and, in a second step, two such neighboring new sites to a new cell (so that the original lattice may be thought of as covered with squares). After restoring, by hand, the original symmetry we find, with p fixed self-consistently, the correct T_c to within 6% and $z=2.03$. If we choose p by adjusting T_c we obtain $z=2.18\pm10\%$ as the mean and the scatter of the values resulting form the two

different sets of recursion relations mentioned.

The average of our three numbers for z in two dimensions is $z_{av}=2.16$; we take it as our "best" one. Their scatter may serve as a measure for the accuracy of our second-order calculation.

For $d=3$, we first form square cells of four neighboring sites in planes and then cubic cells by combining pairs of squares. After restoring the cubic symmetry we get $z=2.24$, $\nu=0.69$, and $K_{1c}=0.26$ (the best available numerical values are $\nu=0.63$ and $K_{1c}=0.22$), if p is fixed self-consistently. For a p that adjusts T_c our results are $z=1.98\pm20\%$ (mean and scatter defined as in the planar case) and $\nu=0.74$.

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