RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 32, NUMBER 9 1 NOVEMBER 1985

Clear evidence of redundant operators in Monte Carlo studies of the Ising model

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(Received 24 July 1985)

After reviewing the notion of redundant operators and the procedure for deriving them analytically for Ising systems, we present Monte Carlo renormalization-group data that clearly show their occurrence as eigenoperators in $d=2$.

In the renormalization-group (RG) approach to critical phenomena[1] one starts with a Hamiltonian $H(\phi)$, subjects it to an RG transformation R_L that reduces the degrees of freedom by a factor L^{-d} (in d dimensions) and gives $H(\phi')$, the effective Hamiltonian for the block-spin[2] variables ϕ'. If H is critical one assumes $R_L^N(H)\rightarrow H^*$ as $N\rightarrow\infty$, while if $H=H^*+\delta H$, R_L is approximated by the linear operator TR_L:

$$\delta H \underset{R_L}{\rightarrow} T_L\delta H \quad . \tag{1}$$

The eigenvalues $\lambda_i=L^{a_i}$ of T_L can be relevant $(a_i>0)$, marginal $(a_i=0)$, or irrelevant $(a_i<0)$, with the same labels attached to the corresponding eigenoperators.

There is, however, yet another class, the *redundant* operators, which usually are relegated to obscurity for three reasons: (i) The nomenclature, which suggests we can live without them. (We will show here it may be very hard to live with them.) (ii) They can be eliminated by a change of variables, and do not affect the free energy. (iii) The associated eigenvalues λ_i can vary from one RG scheme to another and are free of physical significance.

Unfortunately, none of these preclude the possibility of these operators playing havoc in a given Monte Carlo RG (MCRG) study.[3] For example, if any redundant $\lambda_i>1$, $R_L^N(H)$ will not tend to any H^* even if H is critical. Even if $\lambda_i<1$, a_i can mimic a correction-to-scaling exponent.

Pawley *et al.*[4] found such an operator in the odd sector of the $d=3$ Ising model. By use of the ϕ^4 field-theory language they associated it with the ϕ^3 operator which is redundant in that given ϕ, ϕ^2, and ϕ^4 terms, we can generate the ϕ^3 term by shifting: $\phi\rightarrow\phi+\Delta$.

In his detailed article Wegner[5] points out that given any $H(\phi)$ one can generate the redundant operators δH associated with it by making the change $\phi(x)\rightarrow\phi(x)+\delta\phi(x)$. If

$$H=\int \mathscr{H}(\phi)dx \quad , \tag{2}$$

then under

$$\phi\rightarrow\phi+\delta\phi(x) \tag{3}$$

(where $\delta\phi$ depends on x but not ϕ),

$$H\rightarrow H+\delta H \quad , \tag{4}$$

$$\delta H=\int\frac{\partial\mathscr{H}(\phi)}{\partial\phi(x)}\delta\phi(x)dx \quad . \tag{5}$$

It is then easy to show δH is redundant. For example, to show that the partition function is unchanged one proceeds as follows:

$$\begin{aligned} Z(H+\delta H) &= \int d\phi\exp[H(\phi)+\delta H(\phi)] \quad , \\ &= \int d\phi\exp[H(\phi+\delta\phi)] \quad , \\ &= \int d\phi'\exp H(\phi'), \quad \phi'=\phi+\delta\phi \quad , \\ &= Z(H) \quad . \end{aligned} \tag{6}$$

At any point $H(\phi)$ in the space of Hamiltonians all the redundant directions can be derived by choosing all the possible changes of variables $\phi\rightarrow\phi+\delta\phi$. [If $\delta\phi$ depends on ϕ, one must worry about the Jacobian $J(\phi'/\phi)$.] If H is a fixed point, this will be the space that generates the redundant eigenoperators that cloud the issue as described earlier.

This procedure for generating redundant operators runs into a snag when applied to Ising Hamiltonians $H(S)$, $S=\pm1$, since the variables S do not admit an infinitesimal change. The problem was circumvented in Murthy and Shankar[6] as follows. Let us define $H'(S')$ by

$$\begin{aligned} \exp H'(S') &= \sum_s\left[\prod_{\text{sites}}\left(\frac{1+SS'}{2}+\epsilon S'f(S)\right)\right]\exp H(S) \quad , \\ &= \sum_s P(S',S)\exp H(S) \quad . \end{aligned} \tag{7}$$

In the above, $(1+SS')/2=\delta_{SS'}$ is the Kronecker δ for Ising spins, ϵ is a small parameter, and f is any function of the "old spins S." $P(S,S')$ is a projection operator of the type invented by Kadanoff,[7] except that no reduction of degrees of freedom is attempted here. If $\epsilon=0$, clearly $H'=H$. If $\epsilon\neq0$, then $H'=H+\delta H$, where δH is of order ϵ and depends on $f(S)$ *and* H.

Reference 6 shows that this δH is indeed redundant and shows how it may be computed in practice for a given f and H. Several examples were computed for $H=H_{\text{nn}}^*$, the critical nearest-neighbor interaction, in $d=2$ and 3. Even though H_{nn}^* is not the fixed point of any simple RG transformation, it is quite close to the fixed points of many of them. Thus we may expect that the redundant direction at H_{nn}^* approximates very well those of the fixed points H^*. Also, in practice, T_L is diagonalized not at H^* itself, but after some iterations that begin at H_{nn}^*. We will see below that some of the eigenvectors of T_L after one iteration are remarkably close to the redundant operators derived at $H^*_{\rm nn}$.

For $d=2$, in the odd sector, the following short-range redundant operators emerge for $H_{\rm nn}$:

$$\Omega_1 = H_0 + a^2(1-4a+2a^2-4a^3+a^4)^{-1}H_{034} ,$$
$$\Omega_2 = H_0 + 2a^2(1-4a+2a^2-4a^3+a^4)^{-1}H_{012} ,$$
$$\Omega_3 = H_{034} - 2H_{012} = (\Omega_1 - \Omega_2) f(a) , \qquad (8)$$
$$\Omega_4 = H_0 + 2a^3(1-4a+7a^2-16a^3+7a^4-4a^5+a^6)^{-1}H_{135} ,$$
$$\Omega_5 = H_0 + 2a^2(1-4a+4a^2-4a^3+a^4)^{-1}H_{13574} .$$

In the above $a=\tanh K$, and

$$H_{ijk}\ldots = \sum_{\rm sites} (S_iS_jS_k \cdots + \text{rotations and reflections}) , \qquad (9)$$

where the multiplicity at each site is such that any interacting set of spins is represented once and only once. The spins $S_0, S_1, \ldots$ are numbered as follows:

$$\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{bmatrix} . \qquad (10)$$

(The same combination of operators, up to a spin-independent term, occurs in the works of Dekeyser and Rogiers,[8] Lee and Barrie,[9] and Fisher[10] who exploited the symmetry of the measure to obtain relations between correlation functions. Of course these pre-RG analyses did not view them as redundant operators.)

Setting $a=\sqrt{2}-1$ we get the following redundant operators associated with $H^*_{\rm nn}$,

$$\Omega_1 = H_0 - 0.3018 H_{034} ,$$
$$\Omega_2 = H_0 - 0.6036 H_{012} , \qquad (11)$$
$$\Omega_3 = H_{034} - 2H_{012} .$$

We do not discuss Ω_4 and Ω_5 further.

Let us now turn to the data. These were obtained by 2×2 blockings with a majority rule and random tie breakers. The starting H was $H^*_{\rm nn}$ and T_L was evaluated and diagonalized after one blocking. The extraction of T_L was done both á la Swendsen (SW)[11] and Gupta and Corderey (GC).[12] The errors due to truncation in the space of coupling constants will not be discussed here.

Let us consider first the case where only H_0 and H_{034} were kept. Besides the leading right eigenvector $|R_1\rangle$ with eigenvalue 3.681 (Swendsen) or 3.617 (Gupta-Corderey) compared to the expected one, $2^{15/8}=3.6680$, there was a second one:

$$|R_2\rangle = H_0 - 0.3011 H_{034}, \quad \lambda_2 = 0.722 \text{ (SW)} ,$$
$$= H_0 - 0.3115 H_{034}, \quad \lambda_2 = 0.568 \text{ (GC)} . \qquad (12)$$

(The last two digits are not to be taken seriously in view of the various approximations involved.)

It is obvious that R_2 is just $\Omega_1 (=H_0 - 0.3018 H_{034})$. The exponent $a_2 = \ln\lambda_2/\ln 2$ is therefore redundant and could easily have been confused with a correction to scaling exponent. Since the free energy in the presence of a field is unknown, we could not have spotted this problem by any other analytic means.

Note that, in general, a redundant operator derived analytically (as above) need not be a redundant *eigen*operator of some RG. However, in this case of a $2\times2T_L$, the redundant subspace Ω_1 was one dimensional and hence also an eigenspace.

Let us move on to the $3\times3T_L$ which included H_{012}. Equation (8) tells us that there are two linearly independent redundant operators in this space. So we expect two redundant eigenoperators to emerge. Continuity with the 2×2 case tells us that one term will have eigenvalue $\simeq 0.7$ (SW) or 0.6 (GC) and be close to Ω_1. Here, it is,

$$|R_2\rangle = H_0 - 0.2852 H_{034} - 0.0317 H_{012}, \quad \lambda_2 = 0.7257 \text{ (SW)} ,$$
$$= \Omega_1 + 0.0166\Omega_3 + 0.0010 H_{012} . \qquad (13)$$

(In view of all the errors and approximations we must attach no importance to the small H_{012} term. Thus $|R_2\rangle$ lies in the redundant subspace.) Likewise

$$|R_2\rangle = \Omega_1 + 0.0168\Omega_3 - 0.0117 H_{012}, \quad \lambda_2 = 0.6099 \text{ (GC)} . \qquad (14)$$

(The expansion of $|R_2\rangle$ in terms of Ω_1, Ω_2, and a "leftover piece" is not unique; we have chosen to express the leftover piece in terms of H_{012}.)

Finally, the third eigenvector is

$$|R_3\rangle = H_0 - 7.0350 H_{034} + 13.4663 H_{012}, \quad \lambda_3 = 0.0989 \text{ (SW)} ,$$
$$= \Omega_1 - 6.7332\Omega_3 - 0.0010 H_{012} , \qquad (15)$$

and

$$|R_3\rangle = H_0 - 4.4997 H_{0.34} + 8.3495 H_{012}, \quad \lambda_3 = 0.1114 \text{ (GC)} ,$$
$$= \Omega_1 - 4.1979\Omega_3 - 0.0464 H_{012} ,$$

which is consistent with being redundant.

We now move to the even sector in $d=2$. Reference 6 gives two short-range redundant operators at $H^*_{\rm nn}$:

$$\Omega_1 = H_{01} - (\sqrt{2}/3)H_{04} - (\sqrt{2}/6)H_{02} + (1/6\sqrt{2})H_{1357} , \qquad (16)$$
$$\Omega_2 = H_{01} - (2\sqrt{2}/5)H_{04} - (\sqrt{2}/5)H_{02} + (1/10)H_{0124} . \qquad (17)$$

We were not able to see clear evidence for the occurrence of Ω_1 or Ω_2 or a combination thereof as redundant operators. For one thing, in those cases where all the operators in Ω_2 or Ω_2 were included in the analysis, several others were also included. (The MCRG analysis was not tailor made to this study of redundant operators.) The leading eigenvalues 2, 2^{-1}, 2^{-2}, and 2^{-3} were clearly visible. The redundant operators were presumably lower down and severely distorted by the truncation. When we ignored the last terms in Eqs. (16) and (17) and looked for them in the 3×3 case that included H_{01}, H_{04}, and H_{02} we found only the standard eigenvalues 2, 2^{-1}, and 2^{-2}. Presumably the irrelevant eigenvectors, when truncated to this subspace, had bigger eigenvalues than the redundant ones similarly truncated. (Such a thing could also have happened in the odd sector for 2×2 or 3×3 cases if the redundant eigenvalues had been lower than the irrelevant ones.)

We finally turn to the odd sector of the $d=3$ model. Setting $K=0.221\,654$ (suggested by the work of Pawley *et al.*) in the formulas of Ref. 6, we get at $H^*_{\rm nn}$ the following short-range operators:

$$\Omega_1 = H_0 - 0.1740 H_{034} + 0.0362 H_{130^+} , \qquad (18)$$
$$\Omega_2 = H_0 - 0.1160 H_{034} - 0.2320 H_{012} + 0.0241 H_{135} . \qquad (19)$$

The spins are numbered as in $d=2$ except we now need two layers, the upper ones carrying a superscript +. We do not yet have data for this case. So meanwhile we predict that if the redundant operator mentioned by Pawley *et al.*[4] comes from the H_0-H_{034} subspace, it must be close to Ω_1 truncated to that space, i.e., $H_0-0.1740H_{034}$.

The aim of this paper was to emphasize what was evident from the work of Pawley *et al.*, that redundant operators are not curiosities one can turn one's back on, that they can and do play a significant role in numerical studies. We hope that we have done this by demonstrating convincingly that some of the operators that played a major role in the MCRG study of the Ising model were indeed redundant operators by construction.

We are grateful to the J. R. Oppenheimer Foundation (R.G.), to the Alfred P. Sloan Foundation, and to the U.S. Department of Energy, Grant No. DE-AC02-76ERO 3075 (R.S.), for financial support.

[1]K. G. Wilson, Phys. Rev. **84**, 3174 (1971); **84**, 3184 (1971); Rev. Mod. Phys. **47**, 773 (1975); K. G. Wilson and J. B. Kogut, Phys. Rep. **12C**, 75 (1974); M. E. Fisher, in *Critical Phenomena*, edited by F. J. W. Hahne, Lecture Notes in Modern Physics, Vol. 186 (Springer-Verlag, New York, 1983); H. J. Maris and L. P. Kadanoff, Am. J. Phys. **46**, 652 (1978).

[2]L. P. Kadanoff, Rev. Mod. Phys. **39**, 395 (1967).

[3]For a discussion of MCRG, see *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1979), Vol. 7.

[4]G. S. Pawley, R. H. Swendsen, D. J. Wallace, and K. G. Wilson, Phys. Rev. B **29**, 4030 (1984).

[5]F. J. Wegner, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976); J. Phys. C **7**, 2098 (1974).

[6]G. Murthy and R. Shankar, this issue, Phys. Rev. B **32**, 5851 (1985). We thank Professor M. E. Fisher for informing us that K. G. Wilson had discovered some of these tricks for generating redundant operators many years ago. However, this was not published as far as we can tell and as far as Professor K. Wilson can recall.

[7]L. P. Kadanoff, Phys. Rev. Lett. **34**, 1005 (1975); L. P. Kadanoff and A. Houghton, Phys. Rev. B **11**, 377 (1975).

[8]R. Dekeyser and J. Rogiers, Physica **59**, 2 (1972).

[9]K. C. Lee and R. Barrier, Can. J. Phys. **47**, 769 (1969).

[10]M. E. Fisher, Phys. Rev. **113**, 969 (1959).

[11]R. H. Swendsen, Phys. Rev. B **30**, 3866 (1984); **30**, 3875 (1984).

[12]R. Gupta and R. Corderey, Phys. Lett. **105A**, 4151 (1984).