

## Redundant operators for Ising spins

Ganpathy Murthy and R. Shankar

*J. W. Gibbs Laboratory of Physics, Yale University, New Haven, Connecticut 06520*

(Received 17 April 1985)

We remind the reader of the important role that could be played in Monte Carlo renormalization-group studies by redundant operators, defined to be changes in the Hamiltonian due to infinitesimal changes of variables. We then overcome the problem of defining an *infinitesimal* change of variables for discrete Ising spins and construct redundant operators in  $d=2$  and 3. We analyze how they may be seen in numerical experiments.

### I. INTRODUCTION

The Monte Carlo renormalization-group (MCRG) technique is a powerful numerical scheme for studying the critical behavior of statistical mechanical systems or Euclidean field theories on a lattice.<sup>1</sup> By numerical methods one can study the flow of Hamiltonians under renormalization, locate fixed points, measure the eigenvalues of the linearized transformation (i.e., the critical exponents), and so on.

In the numerical studies one expects that if one starts with any critical Hamiltonian  $H_c$ , say critical nearest neighbor (NN), then the flow under renormalization will be towards the fixed point  $H^*$ , while if one begins with a slightly noncritical system, the renormalized  $H$  would initially stay close to the critical surface and move towards  $H^*$  but eventually veer away. This picture stems from the classification of perturbations of  $H^*$  into relevant and irrelevant ones.<sup>2</sup> (We ignore the rare case of truly marginal operators.)

There is, however, another class of operators, namely, *redundant* operators, which can alter this picture. These are defined by Wegner<sup>3</sup> as changes in  $H^*$  when an infinitesimal change of variables is made in the functional integral. To be concrete, consider the example of

$$Z = \int \prod_x d\phi(x) e^{H(\phi(x))} \tag{1.1}$$

Under a change

$$\phi(x) \rightarrow \phi'(x) = \phi(x) + \delta, \tag{1.2}$$

which leaves the measure invariant, we find

$$Z \rightarrow Z' = \int \prod_x d\phi'(x) e^{H(\phi') + \delta H(\phi')} = Z, \tag{1.3}$$

where

$$\delta H(\phi') = - \sum_x \left. \frac{\partial H}{\partial \phi} \right|_{\phi'} \delta. \tag{1.4}$$

The physics is unaffected by the change  $H \rightarrow H + \delta H$ . First, the free energy is unaffected since we can convert  $H + \delta H$  to  $H$  by going backwards from Eq. (1.4) to Eq. (1.1). Secondly, any correlation function  $\langle \phi'_1 \cdots \phi'_n \rangle$  with respect to  $H + \delta H$  has an image in the ensemble generated by  $H$ :

$$\begin{aligned} \langle \phi'_1 \cdots \phi'_n \rangle_{H+\delta H} &= \int \prod_x d\phi'(\phi'_1 \cdots \phi'_n) e^{[H(\phi') + \delta H(\phi')]} \\ &= \int \prod_x d\phi[(\phi_1 + \delta) \cdots (\phi_n + \delta)] e^{H(\phi)} \\ &= \langle (\phi + \delta\phi)_1 \cdots (\phi + \delta\phi)_n \rangle_H, \end{aligned} \tag{1.5}$$

where  $\delta\phi = \delta$ . These ideas generalize readily to case where  $\delta\phi = \delta\phi(x)$ . Each change of variables  $\phi \rightarrow \phi + \delta\phi$  generates its own redundant operator  $\delta H$ .

Let  $H^*$  be the fixed point of some renormalization-group transformation  $R$ . In the vicinity of  $H^*$ , the flow in a redundant direction  $\delta H^*$  is free of physical significance. This is reflected in the fact that the eigenvalue associated with the direction  $\delta H^*$  varies with  $R$ .<sup>3</sup> In the study of Pawley *et al.*<sup>4</sup> an odd operator with a spurious eigenvalue occurred and was identified as a redundant operator. Fortunately, in this case the operator was odd and the flow to a fixed point (restricted to the even sector in MCRG) was not spoiled. On the other hand, one can envisage the possibility of an even redundant eigenvalue which is repulsive. In this case no fixed point will be found if one starts with a critical (NN say) system and generates a flow. The redundant operator is no longer just a curiosity or nuisance.

With the above remarks to motivate a study of redundant operators we ask how to generate them for Ising systems. Whereas for the case of continuous fields  $\phi$  the notion of an infinitesimal change in  $\phi$  (and hence in  $H^*$ ) exists, no obvious candidate exists for Ising spins  $S = \pm 1$ . In  $d=2$ , thinking of Ising systems in terms of continuous fields is not very useful. Besides, MCRG studies are done on  $H(S)$ , and it will be useful to have examples of  $\delta H^*(S)$  that can be interpreted as redundant. These will be constructed in Sec. II. In Sec. III we will consider concrete examples of  $\delta H^*$  in  $d=2$  and 3.

### II. CONSTRUCTION OF REDUNDANT OPERATORS

Consider an Ising system described by

$$Z = \sum_S e^{H(S)} \equiv \sum_S e^{\sum_i S_i V(S_i)}, \tag{2.1}$$

where  $i$  is the site label,  $i$  is any site not equal to  $i$ , and  $V(S)$  is any function. For example, in the case of  $H_{\text{NN}}$ , the nearest-neighbor interaction,  $V = K \sum_j S_j$ , where  $j$  is a NN of  $i$ .

We shall now derive the redundant operators  $\delta H$  for this  $H$ . Of course we are interested in redundant operators  $\delta H^*$  associated with a fixed point  $H^*$ . Since the derivation works for any  $H$ , let us first find  $\delta H$  in general.

As mentioned earlier, the problem with mimicking the derivation of  $\delta H$  associated with  $H(\phi)$  is that in the case of  $H(S)$ ,  $S = \pm 1$ , there is no obvious infinitesimal change of variables  $S \rightarrow S + \delta S$  that respects  $|S| = 1$ . We circumvent this problem as follows.

Let us introduce a matrix  $Q(S', S)$  (where  $S$  and  $S'$  are each collective labels for all the spins) such that

$$\sum_{S'} Q(S', S) = 1. \quad (2.2)$$

Similar functions,  $P(S', S)$ , called projection operators, were introduced to generate block-spin transformations.<sup>5,6</sup> In those cases, however,  $S'$  was defined on a smaller lattice than  $S$ , i.e., one was trying to thin out degrees of freedom. Here we want  $S'$  and  $S$  to be defined on the same lattice. Clearly,

$$\begin{aligned} Z &= \sum_S e^{H(S)} = \sum_{S'S} Q(S', S) e^{H(S)} \\ &= \sum_{S'} e^{H'(S')}. \end{aligned} \quad (2.3)$$

By construction  $S' = \pm 1$ , and  $H'(S')$  is defined by

$$e^{H'(S')} = \sum_S Q(S', S) e^{H(S)}. \quad (2.4)$$

In going from  $H(S)$  to  $H'(S')$  we have preserved the partition function, the lattice size, and the condition

$$\begin{aligned} e^{H'(S')} &= e^{H(S)} \left[ 1 + \epsilon \sum_i \sum_{S'_i} S'_i [f_1(S'_i) + S_i f_2(S'_i)] e^{(S_i - S'_i)V(S'_i)} \right] \\ &= e^{H(S)} \left[ 1 + \epsilon \sum_i S'_i e^{-S'_i V(S'_i)} \{ 2f_1(S'_i) \cosh[V(S'_i)] + 2f_2(S'_i) \sinh[V(S'_i)] \} \right] \\ &\equiv e^{H(S') + \delta H(S')}, \end{aligned} \quad (2.11)$$

which gives us

$$\begin{aligned} \delta H(S') &= 2\epsilon \sum_i S'_i e^{-S'_i V(S'_i)} [f_1(S'_i) \cosh V(S'_i) \\ &\quad + f_2(S'_i) \sinh V(S'_i)]. \end{aligned} \quad (2.12)$$

Before considering explicit examples of  $\delta H$ , let us present the evidence that these are indeed redundant operators associated with  $H$ . First, they are generated by a change of coordinates  $S \rightarrow S'$  and they do not affect  $Z$  (to first order in  $\epsilon$ , just as is required in the case of continuous fields also) or the lattice size. The sum of any two redundant operators is redundant, as can be seen by compounding

$|S| = 1$ , all of which allow us to view the change  $H \rightarrow H'$  as the result of a change of variables. To generate an infinitesimal transformation we start with the identity transformation

$$I = \prod_i \left[ \frac{1 + S'_i S_i}{2} \right] \equiv \prod_i \delta(S'_i, S_i) \quad (2.5)$$

and add an infinitesimal generator:

$$Q_\epsilon = \prod_i [\delta(S'_i, S_i) + \epsilon S'_i f(S)]. \quad (2.6)$$

Here  $f(S)$  is any function of the "old" spins  $S$ , and the  $S'_i$  in front of  $f$  ensures Eq. (2.2) is valid. We then have

$$\begin{aligned} e^{H'(S')} &= \sum_S \prod_i [\delta(S'_i, S_i) + \epsilon S'_i f(S)] e^{H(S)} \\ &= e^{H(S')} + \epsilon \sum_i \sum_S \left[ \prod_i \delta(S'_i S_i) \right] S'_i f(S) \\ &\quad \times e^{H(S_i, S_i)} + O(\epsilon^2). \end{aligned} \quad (2.7)$$

Let us expand  $f(S)$  as

$$f(S) \equiv f(S_i, S_i) = f_1(S_i) + S_i f_2(S_i) \quad (2.8)$$

and define

$$\Delta H = H(S_i, S'_i) - H(S'_i, S'_i) \quad (2.9)$$

$$= (S_i - S'_i) V(S'_i), \quad (2.10)$$

where  $V$  stands for the terms coupled to the spin at  $i$  [see Eq. (2.1)]. Then

the infinitesimal transformation associated with each. For the case  $H = H_{\text{NN}}^*$ , the critical nearest-neighbor system with  $K = \tilde{K} = -\frac{1}{2} \text{Intanh} K$ , we have verified for the various cases we studied that  $H_{\text{NN}}^* + \delta H_{\text{NN}}^*$  lies on the critical surface (CS) by using our earlier work<sup>7</sup> where the equation for the CS near  $H_{\text{NN}}^*$  was derived. (This test is useful because it eliminates operators  $\Delta H$  which keep  $Z$  the same to first order because  $\langle \Delta H \rangle = 0$ , but which take us out of the CS. These cannot be called redundant since they change by physics, i.e., the correlation length. The redundant  $\delta H$  are characterized by the fact that they are linear combinations of interactions with coefficients *analytic* in the parameters of  $H$ .) Next we would like to establish the analog of Eq. (1.5). Consider, for example,

$$\begin{aligned}
\langle S'_1 S'_2 \rangle_{H+\delta H} &= Z^{-1} \sum_{S'} \sum_S S'_1 S'_2 \left[ \prod_i [\delta(S_i, S'_i) + \epsilon S'_i f(S)] \right] e^{H(S)} \\
&= \langle S_1, S_2 \rangle_H + Z^{-1} \epsilon \sum_{SS'} \sum_i \left[ \prod_i \delta(S_i, S'_i) \right] S'_i f(S) e^{H(S)} S'_1 S'_2 + O(\epsilon^2). \quad (2.13)
\end{aligned}$$

The first term comes from taking the  $\delta$  from each site and doing the sum over  $S'$  first, while the second comes from taking  $\delta$  at all sites but one where  $\epsilon S' f$  is taken instead. Consider a given value of  $i$ . If we sum over  $S'_i$  we will get 0 (because of the factor  $S'_i$ ) unless  $S'_1$  or  $S'_2$  gets rid of it, i.e., unless  $i=1$  or  $2$ . It is evident that

$$\begin{aligned}
\langle S'_1 S'_2 \rangle_{H+\delta H} &= \langle S_1, S_2 \rangle_H + \langle \epsilon f(S)_1, S_2 \rangle_H + \langle S_1, \epsilon f(S)_2 \rangle_H \\
&= \langle [S + \epsilon f(S)]_1, [S + \epsilon f(S)]_2 \rangle_H. \quad (2.14)
\end{aligned}$$

Thus the correlation functions transform as if the change  $S \rightarrow S + \epsilon f(S)$  has been made. We say "as if", because the literal change  $S \rightarrow S + \epsilon f(S)$  cannot be made without violating  $|S|=1$ . For those readers who would like to see redundant operators arising from a literal infinitesimal change of variables (as in the case of  $\phi$ ) we provide the following alternate version, which for practical reasons is limited to the case  $H_{NN}$ . Let us work with the transfer matrix  $T(\sigma)$ , written in terms of Pauli matrices such that

$$A = \text{Tr} T^R,$$

where  $R$  is the number of rows (in  $d=2$ ) or layers (in  $d=3$ ). The trace is originally taken in the eigenbasis of  $\sigma_3$ , the eigenvalues  $\pm S$  being the spins summed over in the nonoperator version. However, as the trace can be taken in any basis related by a unitary transformation  $U$ , let us take it in the basis of  $\tilde{\sigma} = U^\dagger \sigma U$ . Let us now express every  $\sigma$  in  $T$  in terms of  $\tilde{\sigma}$ . This amounts to making an infinitesimal (operator) change of variables  $\sigma \rightarrow \sigma + \delta\sigma$ , where  $\delta\sigma = i\epsilon[\Omega, \sigma]$  for the case  $U = I + i\epsilon\Omega$ . (We restrict ourselves to unitary rather than similarity transformations since we want  $\tilde{\sigma}$  to be isomorphic to  $\sigma$  and, in particular, Hermitian.) Under this change

$$T \rightarrow UTU^\dagger = T + \Delta T = T(1 + \epsilon\rho).$$

If we now go back to  $S$  language,  $\epsilon\rho$  will correspond to the additional interaction  $\delta H_{NN}$  which is clearly redundant. In Appendix A we give a concrete example of such a  $\delta H$  for  $d=2$  and it agrees with the redundant  $\delta H$  found via Eq. (2.12) for a certain choice of  $f$ . The transfer-matrix approach is much more cumbersome and for practical reasons limited to  $\delta H_{NN}$ . It is presented here only to corroborate the fact that what we are doing indeed corresponds to a change of variables.

Finally, we would like to show that if  $\delta H^*$  is redundant, then under any RG transformation it goes into  $\delta H'^*$ , which is also redundant in the sense that  $\delta H'^*$  is generated from  $H^*$  by a change of variables.

Consider a vector  $V(H)$  which has  $2^N$  components labeled by the spins  $S$  on a lattice with  $N$  sites, and having values

$$V_S(H) = e^{H(S)}. \quad (2.15)$$

We may view  $Q_\epsilon$  Eq. (2.6) as a square ( $2^N \times 2^N$ ) matrix in this space:

$$V_{S'}(H') = \sum_S Q_{S'S} V_S(H),$$

or in an compact notation

$$V(H') = QV(H). \quad (2.16)$$

Although  $Q$  acts linearly on  $V$  the action on  $H$  is nonlinear. To find  $Q:H \rightarrow H'$ , we must start with  $V_S(H)$ , transform by  $Q$ , extract the couplings from  $V_{S'}(H')$ , and reconstruct  $H$ . (This can be done since there are  $2^N$  known Boltzmann weights and  $2^N$  interactions.) The usual block-spin transformation generated by  $P(S', S)$  is represented in this notation as

$$V'(H') = PV(H), \quad (2.17)$$

where  $P$  is a rectangular matrix with  $2^{N/L^2}$  rows and  $2^N$  columns where  $L$  is the "block size," i.e.,  $L^2$  equals the number of spins after divided by the number of spins before.

As the matrix  $P$  becomes infinitely large, the fact that  $V(H)$  can carry more interactions than  $V'(H')$  becomes unimportant. If  $H^*$  is a fixed point of  $P$ , we cannot of course say  $V'(H^*) = V(H^*)$  since they have different dimensions, but we can say that if  $H'$  is extracted from  $V'$ , it agrees with the  $H^*$  put into  $V$  for all couplings of finite range.

If we start with  $V(H^*)$  and let  $Q = I + \epsilon F$  act on it, it produces a redundant change

$$\Delta V(H^*) = \epsilon FV(H^*). \quad (2.18)$$

We wish to show that if one implements a blocking  $P$  [which takes  $V(H^*)$  to  $V'(H^*)$ ] on  $V(H^*) + \Delta V(H^*)$ , the result is  $V'(H^*) + \Delta V'(H^*)$ , where  $\Delta V'(H^*) = \epsilon F'V'(H^*)$  where  $F'$  is some generator, like  $F$ . Therefore, let us consider

$$\begin{aligned}
P(V + \Delta V) &= PV(H^*) + P\Delta V(H^*) \\
&= V'(H^*) + \epsilon PFV(H^*) \\
&\equiv V'(H^*) + \Delta V'(H^*). \quad (2.19)
\end{aligned}$$

Therefore,

$$\Delta V'(H^*) = \epsilon PFV(H^*). \quad (2.20)$$

Suppose we can write

$$PF = F'P \quad \text{for some } F', \quad (2.21)$$

then

$$\begin{aligned}
\Delta V'(H^*) &= \epsilon F'PV(H^*) \\
&= \epsilon F'V'(H^*), \quad (2.22)
\end{aligned}$$

i.e.,  $\Delta V'(H^*)$  is the redundant change produced by the generator  $\epsilon F'$ . If we set  $2^N = M$ ,  $2^{N/L^2} = m$ , then  $Q$  is  $M \times M$ ;  $P$  is  $m \times M$ ;  $F$  is  $M \times M$ ,  $F'$  is  $m \times m$ . Equation (2.21) can be solved for  $F'$ :

$$F' = PFP^{-1}, \quad (2.23)$$

where  $P^{-1}$  is the right inverse of  $P$ . There is no problem constructing such an inverse; in fact, there is an infinite number of them since  $P$  corresponds to  $m$  equations among  $M$  unknowns. (We are making the mild assumption that the  $m$  rows of  $P$  are linearly independent.) Different choices of  $F'$  will correspond to different changes of variables, but  $\Delta V'$  generated by them will be the same in all cases since they differ by the annihilators of  $V'$ . One can also check that  $Q' = I + \epsilon F'$  obeys Eq. (2.2), i.e.,

$$\sum_{S'} Q'(S', S) = 1$$

or

$$\sum_{S'} F'(S', S) = 0.$$

### III. CONCRETE EXAMPLES

Let us return to Eq. (2.12) and generate different examples of  $\delta H$  by choosing  $f_1$  and  $f_2$  at will. First, let us note that in Eq. (2.12) the quantity in brackets is just some function  $A(S_i)$ . The breakdown into  $f_1$  and  $f_2$  will no longer interest us since we do not want to follow the change of correlation functions as per Eq. (2.14). Therefore, we write

$$\delta H = \epsilon \sum_i S_i e^{-S_i V(S_i)} A(S_i); \quad (3.1)$$

written this way,  $\delta H$  coincides with Eq. (3) of Dekeyser and Rogiers,<sup>8</sup> who derived linear relations between correlation functions by finding operators  $X$  for which  $\langle X \rangle = 0$  due to the symmetry of the measure. Such relations which also occurred elsewhere<sup>9,10</sup> were, however, not seen as resulting from infinitesimal transformations, and  $X$  was not viewed as a redundant operator.

Since we are interested in a  $\delta H^*$  associated with a fixed point  $H^*$ , we must first pick our  $H^*$  and then each

$$\delta H_1 = (1 - 6a)A + a^2B + a^2C - a^3D - a^3E + a^4F + a^4G - a^5H + a^6M, \quad (3.4a)$$

$$\delta H_2 = (a^2 - 2a - 4a^3)A + (1 + 6a^2 + 5a^4)B/12 + (2a^2 + a^4)C/3 - (2a + 8a^3 + 2a^5)D/12 - (2a + 4a^3 + 2a^5)E/8 + (a^2 + 2a^4)F/3 + (5a^2 + 6a^4 + a^6)G/12 - (4a^3 + 2a^5)H/6 + a^4M, \quad (3.4b)$$

$$\delta H_3 = (-2a + a^2 - 4a^3)A + (8a^2 + 4a^4)B/12 + (1 + 2a^4)C/3 - (4a + 4a^3 + 4a^5)D/12 - 8a^3E/8 + (2a^2 + a^6)F/3 + (4a^2 + 8a^4)G/12 - (4a^3 + 2a^5)H/6 + a^4M,$$

where  $a = \tanh K$  and should be set equal to  $\tanh(0.221654)$  to get  $\delta H^*$ . There are three more such operators  $\delta H_4$ ,  $\delta H_5$ , and  $\delta H_7$  obtained by changing  $a \rightarrow 1/a$  and multiplying by  $a^6$ .

The operators  $A-M$  are defined as follows. Imagine spins numbered in a plane as in Appendix A [following Eq. A19] with an identical layer above, numbered  $0^+$

choice of  $A$  will generate a redundant operator. Clearly the simpler  $H^*$  and  $A$  are, the simpler  $\delta H^*$  will be. We will choose  $H^* = H_{NN}$ , the critical nearest-neighbor interaction first in  $d=2$  and then in  $d=3$ . Although  $H_{NN}^*$  is not the fixed point for the usual  $2 \times 2$  or  $3 \times 3$  blockings,<sup>11,12</sup> Swendsen has shown<sup>13</sup> that "optimized" RG transformations for which this is the fixed point do exist.

In  $d=2$ , if we want redundant operators involving just the coupling of any spin and its four nearest neighbors, we can choose

$$A = A_{\alpha\beta\gamma\delta} = S_1^\alpha S_2^\beta S_3^\gamma S_4^\delta,$$

where  $S_1, \dots, S_4$  are the four neighbors and  $\alpha$  through  $\gamma=0$  or  $1$ . These 16 relations yield (upon using various symmetries) six redundant operators which are listed in Ref. 8. We mention just the even ones here:

$$\delta H_1 = \epsilon \sum_{\text{sites}} [S^3 H_{1357} + 2C(2C^2 - 1)H_{01} - 2SC^2 H_{04} - SC^2 H_{02} - S(3C^2 - 1)], \quad (3.2a)$$

where  $C = \cosh(2K)$  and  $S = \sinh(2K)$ , so that at  $K = 0.44068\dots$ ,

$$\delta H_1^* = \epsilon \sum_{\text{sites}} (H_{1357} + 6\sqrt{2}H_{01} - 4H_{04} - 2H_{02} - 5), \quad (3.2b)$$

$$\delta H_2 = \epsilon \sum [(C^3 + 2S^2C + C)H_{01} - 2C^2SH_{04} + \frac{1}{2}S^2CH_{0124} - SC^2H_{02} - 2C^2S], \quad (3.3a)$$

which implies

$$\delta H_2^* \equiv \epsilon \sum (5\sqrt{2}H_{01} - 4H_{04} + 2^{-1/2}H_{0124} - 2H_{02} - 4). \quad (3.3b)$$

The convention for the naming and normalization of these operators  $H_{ijk\dots}$  is given in Appendix A following Eq. (A19). Note incidentally that the  $\delta H$  in Eq. (A19), derived in the transfer-matrix approach, agrees with  $\delta H_2$  above.

In  $d=3$  we shall focus on odd redundant operators since one may have been seen in numerical studies.<sup>4</sup> Here are six with the shortest possible ranges of interactions:

through  $9^+$ . Then  $A = H_0$ ,  $B = H_{013}$ ,  $C = H_{012}$ ,  $D = H_{135}$ ,  $E = H_{130^+}$ ,  $F = H_{13457}$ ,  $G = H_{01241^+}$ ,  $H = H_{13574^+}$ , and  $M$  is the product of a spin with its six nearest neighbors. The multiplicity of each term is as in  $d=2$ . For example, there are 12 terms per site implied in  $D$  or  $G$ , eight per site in  $E$ , etc.

By forming linear combinations of these operators we can get new ones involving just three or four:

$$\begin{aligned} \delta H_7 = & (1 - 6a + 3a^2 - 12a^3 + 3a^4 - 6a^5 + a^6)a^{-2}A \\ & + (1 + a^2)B - aE, \end{aligned} \quad (3.5)$$

$$\begin{aligned} \delta H_8 = & (1 - 6a + 3a^2 - 12a^3 + 3a^4 - 6a^5 + a^6)a^{-2}A \\ & + 2(1 + a^2)B/3 + 4(1 + a^2)C/3 - 2aD/3. \end{aligned} \quad (3.6)$$

Now that we have a few short-range redundant operators, can we ask how they tie in with the numerical work? This turns out to be a difficult question. First of all, we do not have redundant eigenvectors, simply redundant operators. Next, we have no idea what the redundant eigenvalues will be since they depend on the optimized transformations that make  $H_{\text{NN}}^*$  the fixed point. Lastly, in the numerical work one finds the eigenvectors and eigenvalues of  $T_{\alpha\beta}$ , which is the linearized transformation matrix  $T^\infty$  truncated to a finite-dimensional subspace of interactions. The connection between the solution to this problem and that of the exact one in infinite dimensions is unclear. Also, given that in practice one must work with a finite number of couplings, say 15, it is not clear which 15 to choose to get the leading eigenvalues. For the physical (i.e., relevant and irrelevant couplings) there is reason to believe that one must start within the shortest-range couplings and work upwards in range, i.e., the belief is that the leading eigenvectors will be saturated by a few short-range interactions and hence recovered without much mutilation in a small subspace calculation. We do not know if this applies to the unphysical redundant ones, although it seems plausible in momentum space renormalization.

In view of all this we can say only the following. Consider the even redundant operators  $\delta H_1^*$  and  $\delta H_2^*$  in  $d=2$ . We know from the exact solution that all irrelevant eigenvalues are integers. If the eigenvalue problem of  $T^\infty$  is solved any noninteger eigenvalue must be associated with a redundant operator. If the eigenvector is saturated by short-range couplings one can reasonably hope to see it as an eigenvector of the truncated  $T_{\alpha\beta}$ . The only way in practice that we will know this is happening is that as  $T_{\alpha\beta}$  is made larger, the eigenvector and eigenvalue remain stable. If the vector lies in the subspace  $H_{1357}, H_{01}, H_{04}$ , and  $H_{02}$ , we can expect it to be close to  $\delta H_1^*$  [Eq. (3.2b)]; if it lies in the space  $H_{01}, H_{04}, H_{0124}$ , and  $H_{02}$  it will be close to  $\delta H_2^*$ ; and if it involves all of the above interactions it must be a linear combination of  $\delta H_1^*$  and  $\delta H_2^*$ . Conversely, any eigenvector (stable under enlargement of  $T_{\alpha\beta}$ ) that lies in this subspace must be linearly independent of  $\delta H_1^*$  and  $\delta H_2^*$  if the corresponding eigenvalue is an integer. It is also clear that we must work in spaces involving the above couplings before a redundant operator could possibly enter.

What if no redundant eigenvectors (i.e., noninteger eigenvalues) are found if  $T_{\alpha\beta}$  is studied in the space of the  $H$ 's mentioned above? Then we would have to conclude that  $\delta H_1^*$  and  $\delta H_2^*$  are nowhere near being eigenvectors of

$T^\infty$ , and that they are linear combinations of eigenvectors which are predominantly outside the subspace in question. (We are ignoring the freak case of a redundant eigenvalue being accidentally integer.)

In  $d=3$ , if a stable odd repulsive eigenvector besides the leading one is found, and it is saturated by short-range couplings, we can expect it to be a linear combination of the six  $\delta H$ 's given earlier. It must also be true that the leading relevant one is linearly independent of these.

#### IV. CONCLUSION

We have shown that redundant operators can be derived for discrete spins despite the fact that there seems to be no obvious way to perform an infinitesimal change of variables. Although a literal infinitesimal change is still out of the question, we found a way to induce infinitesimal transformations in which  $H$  is changed by an infinitesimal amount  $\delta H$ . We showed that the  $\delta H$ 's so obtained met all the tests for redundancy: They formed a subspace, they left the physics invariant, they were closed under renormalization.

*Note added in proof.* For clear evidence of redundant operators (that were derived by these methods) occurring in the odd sector in  $d=2$ , see Ref. 14.

#### ACKNOWLEDGMENTS

We thank Professor R. Swendsen for useful conversations. This work was funded by the Alfred P. Sloan Foundation (R.S.) and U.S. Department of Energy Grant No. DE-AC02-76ER0 3075.

#### APPENDIX A

Here we will derive a redundant operator associated with  $H_{\text{NN}}$  in  $d=2$  in the transfer-matrix formalism. As explained earlier the chief attraction of this approach is that a literal, infinitesimal change of (operator) variables generates  $\delta H$ .

Let us first write (for general  $K$ ) the partition function on a lattice with  $M$  rows and  $N$  columns (numbered by integers  $m$  and  $n$ , respectively) in terms of the transfer matrix  $T$ :

$$Z = [2 \sinh(2K)]^{M/2} \text{Tr} T^M, \quad (A1)$$

$$T = \exp \left[ K \sum_n \sigma_3(n) \sigma_3(n+1) \right] \exp \left[ \tilde{K} \sum_n \sigma_1(n) \right]. \quad (A2)$$

Here  $\tilde{K} = -\frac{1}{2} \ln \tanh K$  and  $\sigma(n)$  are the Pauli matrices at the sites of a one-dimensional lattice labeled by the integer  $n$ . The sum over  $S$  in  $Z$  is now viewed as the trace over the combined eigenvalues of the  $\sigma_3(n)$ 's. We now replace the sum over  $S$  by the sum over  $S'$  (again  $= \pm 1$ ) which are the eigenvalues of the transformed operators

$$\tilde{\sigma}_3(n) = U^\dagger \sigma_3(n) U. \quad (A3)$$

This leaves  $Z$  invariant since the trace is invariant under a unitary change of basis. If we now replace all the  $\sigma$ 's by  $\tilde{\sigma}$ 's in  $T$  and reconstruct the new Boltzmann weights we

will find these correspond to  $H_{NN}(S') + \delta H(S')$ . Since  $U$  can be chosen close to the identity

$$U = I + i\epsilon\Omega \quad (\Omega = \Omega^\dagger), \quad (\text{A4})$$

$\delta H(S')$  will really be infinitesimal and redundant by construction. At the end we will of course set  $K = \tilde{K}$ , the critical value, to get the redundant operator for  $H_{NN}^*$ .

To illustrate our procedure we choose

$$\Omega = \sum_n \sigma_2(n)\sigma_3(n+1). \quad (\text{A5})$$

Under the action of  $\Omega$ ,  $T$  changes as follows:

$$\begin{aligned} T &\rightarrow UTU^\dagger \\ &= T + i\epsilon[\Omega, T] \\ &= (1 + i\epsilon T^{-1}[\Omega, T]) \\ &= T[I + \epsilon(T^{-1}\Omega T - \Omega)] \\ &\equiv T[1 + \epsilon\rho]. \end{aligned} \quad (\text{A6})$$

In order to calculate

$$\rho = i[T^{-1}\Omega T - \Omega] \equiv i\hat{\Omega} - i\Omega, \quad (\text{A7})$$

we shall exploit the linear relation between  $\rho$  and  $\Omega$ . We will first calculate  $\rho$  due to just one term in Eq. (A5), with  $n=0$ ; and then do the sum over  $n$  in the answer so obtained. In terms of  $\sigma \equiv \sigma(0)$ ,  $\bar{\sigma} = \sigma(-1)$ ,  $\sigma' = \sigma(1)$ ,

$$\rho = i\hat{\sigma}_2\hat{\sigma}_3' - i\sigma_2\sigma_3', \quad (\text{A8})$$

where

$$\hat{\sigma} = T^{-1}\sigma T. \quad (\text{A9})$$

Consider first

$$-i\sigma_2\sigma_3' = \sigma_1\sigma_3\sigma_3'. \quad (\text{A10})$$

Now one can check,<sup>15</sup> by computing  $\hat{\sigma}_3 = T^{-1}\sigma_3 T$ , that

$$\sigma_1 = (C - S\hat{\sigma}_3\sigma_3), \quad (\text{A11})$$

where

$$C = \cosh 2K, \quad S = \sinh 2K. \quad (\text{A12})$$

Setting this into Eq. (A10), we get

$$-i\sigma_2\sigma_3' = C\sigma_3\sigma_3' - S\hat{\sigma}_3\sigma_3'. \quad (\text{A13})$$

Our motivation for writing everything in terms of  $\sigma_3$  and  $\hat{\sigma}_3$  is that one can read off the corresponding change  $\delta H$  in the Ising interaction by inspection. For illustration let us consider the  $d=1$  case. Let  $E_0(S', S)$  be the energy of two adjacent "rows" with spins  $S'$  and  $S$ . Then the transfer matrix  $T$  obeys

$$\exp E_0(S', S) = \langle S' | T | S \rangle. \quad (\text{A14})$$

Let us now add a term  $\epsilon E(S', S)$  to  $E_0$ . The new  $T$  given by  $T(1 + \epsilon\rho)$  obeys

$$\exp[E_0(S', S)][1 + \epsilon E(S', S)] = \langle S' | T(1 + \epsilon\rho) | S \rangle, \quad (\text{A15})$$

so that

$$\exp E_0(S', S) E(S', S) = \langle S' | \epsilon T \rho | S \rangle. \quad (\text{A16})$$

Let  $E(S', S) = a(S + S') + bSS'$ . We can get all these terms to occur on the right-hand side by replacing every  $S$  by a  $\sigma_3$  acting to the right on  $|S\rangle$  and every  $S'$  by a  $\sigma_3$  acting to the left on  $\langle S'|$ . For example,

$$\begin{aligned} e^{E_0(S', S)} S' S &= S' S \langle S' | T | S \rangle = \langle S' | \sigma_3 T \sigma_3 | S \rangle \\ &= \langle S' | T T^{-1} \sigma_3 T \sigma_3 | S \rangle \\ &= \langle S' | T \hat{\sigma}_3 \sigma_3 | S \rangle. \end{aligned} \quad (\text{A17})$$

Conversely a term  $\epsilon \hat{\sigma}_3 \sigma_3$  in  $\epsilon\rho$  translates into an interaction  $\epsilon S' S$ . The extension to  $d=2$  (or 3) is direct, one lets  $S'$  and  $S$  be a shorthand for the spins in two adjacent rows (or layers). Given all this we can see that Eq. (A13) translates into the following interaction among the Ising spins (if we remember to reinstate the sum over  $n$ ):

$$\delta H = \sum_{\text{sites}} (CS_{n,m}S_{n,m+1} - SS_{n+1,m}S_{n,m+1}). \quad (\text{A18})$$

We must next treat the first term in Eq. (A8),  $i\hat{\sigma}_2\hat{\sigma}_3$ , in a similar fashion, expressing all operators in terms of  $\hat{\sigma}_3$ 's and  $\sigma_3$ 's, with all quantities with carets on the left. In this "normal ordered" form, the classical interaction can be read off by inspection. The final outcome of the calculation (relegated to Appendix B) is that

$$\begin{aligned} \delta H &= \epsilon \sum_{\text{sites}} [(C^3 + 2S^2C + C)H_{01} - 2C^2SH_{04} \\ &\quad + \frac{1}{2}S^2CH_{0124} - SC^2H_{02} - 2C^2S]. \end{aligned} \quad (\text{A19})$$

The interaction  $H_{0124}$ , for example, stands for a coupling  $S_0S_1S_2S_4$  in the following notation:

$$\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{bmatrix},$$

as well as three other terms (per site) obtained by rotating and reflecting the triangle 0124. Likewise  $H_{02}$  stands for the coupling  $S_0S_2$  and its partner related by a  $+90^\circ$  rotation. (The multiplicity of each term is such that each interacting pair or quartet of spins is represented once and once only when the sum over sites is carried out.)

The careful reader may ask how we could get a coupling between two spins that are separated by two sites in the  $y$  direction when our transfer-matrix formalism can accommodate only coupling between adjacent rows. The answer is that the  $\Omega$  we began with only generates the coupling  $S_0S_2$  but not its partner,  $S_6S_0$ . Likewise it only generates the triangle 0124 but not its three companions. Thus if we imagine  $H_{NN}$  embedded in a space of generally anisotropic couplings,  $\Omega$  generates a redundant direction  $\delta H_\Omega$  that points in the space of anisotropic (but translationally invariant) interactions. What this means is that if one perturbs  $H_{NN}$  with anisotropic terms and carries out the isotropic RG of Swendsen, one of the directions,  $\delta H_\Omega$ , is redundant. Suppose we repeat the analysis using an  $\Omega'$  which is obtained by reflecting  $\Omega$  about a column. This will generate  $\delta H_{\Omega'}$  which is related to  $\delta H_\Omega$

by the same reflection since  $T$  is reflection symmetric. Since the sum of two redundant operators is also redundant,  $\delta H_\Omega + \delta H'_\Omega$  is also a redundant operator. Likewise if we use the column-to-column transfer matrix we will generate a  $\delta H$  that will be related to  $\delta H_\Omega$  by a  $90^\circ$  rotation. More generally, we could argue that given a  $\delta H_\Omega$  which is redundant, there must be other redundant operators related to it by the symmetries of  $H^*$  and the RG transformation. The sum of all such operators will then be redundant and lie in the space of symmetric interactions. This is what is given by Eq. (A19). Finally, we must put  $C = \sqrt{2}$  and  $S = 1$  to get  $\delta H^*$ , the redundant operator associated with  $H_{NN}^*$ .

#### APPENDIX B

Here we convert the term  $i\hat{\sigma}_2\hat{\sigma}'_3$  in  $\rho$  [Eq. (A8)] to a classical interaction by expressing everything in terms of  $\hat{\sigma}_3$ 's and  $\sigma_3$ 's, with all quantities with carets situated to the left. Therefore, let us begin with

$$i\hat{\sigma}_2\sigma'_3 = \hat{\sigma}_3\hat{\sigma}_1\hat{\sigma}'_3 \quad (\text{B1})$$

and try to eliminate  $\hat{\sigma}_1$ . Since  $\sigma_1 \equiv \sigma_1(0)$ ,

$$\hat{\sigma}_1 = T^{-1}\sigma_1 T = e^{-\tilde{K}\sum\sigma_1} e^{-K(\sigma_3\sigma'_3 + \sigma_3\bar{\sigma}_3)} \times \sigma_1 e^{K(\sigma_3\bar{\sigma}_3 + \sigma_3\sigma'_3)} e^{\tilde{K}\sum\sigma_1} \quad (\text{B2})$$

If we now use relations like

$$e^{K\sigma_3\sigma'_3} = \cosh K + \sigma_3\sigma'_3 \sinh K \quad (\text{B3})$$

[because  $(\sigma_3\sigma'_3)^2 = 1$ ] we get

$$\hat{\sigma}_1 = e^{-\tilde{K}\sum\sigma_1} (C^2\sigma_1 + SC\sigma_1\sigma_3\bar{\sigma}_3 + SC\sigma_1\sigma_3\sigma'_3 + S^2\sigma_1\bar{\sigma}_3\sigma'_3) e^{\tilde{K}\sum\sigma_1} \quad (\text{B4})$$

When we take  $\exp(-\tilde{K}\sum\sigma_1)$  through the parentheses and pair it with  $\exp(\tilde{K}\sum\sigma_1)$ , (i) it leaves all  $\sigma_1$ 's alone, and (ii) replaces every  $\sigma_3$ ,  $\bar{\sigma}_3$ , and  $\sigma'_3$  by  $\hat{\sigma}_3$ ,  $\hat{\sigma}_3$ , and  $\hat{\sigma}'_3$  since as far as these are concerned, it is like taking  $T^{-1}$  through the parentheses and pairing it with  $T$ .

We next feed this expression with carets in the right places back in Eq. (A8), eliminate  $\sigma_1$  using

$$\sigma_1 = C - S\hat{\sigma}_3\sigma_3, \quad (\text{B5})$$

and take all quantities with carets on the left using

$$[\hat{\sigma}_3, \sigma'_3, \text{ or } \hat{\sigma}_3] = 0, \quad [\sigma_3(n), \hat{\sigma}_3(m)] = 0, \quad m \neq n \quad (\text{B6})$$

$$\sigma_3\hat{\sigma}_3 = -\hat{\sigma}_3\sigma_3 + 2C/S,$$

and read off the classical interaction. Finally, we add the two terms coming from the second piece,  $-i\sigma_2\sigma'_3$  in Eq. (A8) for  $\rho$ , symmetrize the expression using reflections, rotations, etc., to get Eq. (A19).

<sup>1</sup>For a discussion of MCRG, see *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin, 1979), Vol. 7.

<sup>2</sup>K. G. Wilson, Phys. Rev. B **4**, 3174 (1971); **4** 3184 (1971); K. G. Wilson and J. B. Kogut, Phys. Rep. **12C**, 75 (1974); M. E. Fisher, in *Critical Phenomena*, proceedings of the Summer School at the University of Stellenbosch, edited by F. J. W. Hahne (Springer, Berlin, 1976).

<sup>3</sup>F. J. Wegner, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.

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

<sup>5</sup>L. K. Kadanoff, Phys. Rev. Lett. **34**, 1005 (1975); L. P. Kadan-

off and A. Houghton, Phys. Rev. B **11** 377 (1975).

<sup>6</sup>For a review, see Th. Niemeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.

<sup>7</sup>G. Murthy and R. Shankar, Phys. Rev. Lett. **54**, 1110 (1985).

<sup>8</sup>R. Dekeyser and J. Rogiers, Physica **59**, 2 (1972).

<sup>9</sup>K. C. Lee and R. Barrie, Can. J. Phys. **47**, 769 (1969).

<sup>10</sup>M. E. Fisher, Phys. Rev. **113**, 969 (1959).

<sup>11</sup>R. H. Swendsen, Phys. Rev. B **30**, 3866 (1984); **30**, 3875 (1984).

<sup>12</sup>R. Gupta and R. Cordery, Phys. Lett. **1054**, 415, (1984).

<sup>13</sup>R. H. Swendsen, Phys. Rev. Lett. **52**, 2321 (1984).

<sup>14</sup>R. Shankar and R. Gupta, Phys. Rev. B **32**, 6090 (1985).

<sup>15</sup>C. Itzykson, Nucl. Phys. **B210**, 448 (1982).