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Variational Approximations for Renormalization Group Transformations

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Approximate recursion relations which give upper and lower bounds on the free energy are described. Optimal calculations of the free energy can then be obtained by treating parameters within the renormalization equations variationally. As an example, a particularly simple lower bound approximation which preserves the symmetry of the Hamiltonian (the one-hypercube approximation) is described. The approximation is applied to both the Ising model and the Wilson–Fisher model. At the fixed point a parameter is set variationally and critical indices are calculated. For the Ising model the agreement with the exact results at $d = 2$ is surprisingly good, 0.1%, and is good at $d = 3$ and even $d = 4$. For the Wilson–Fisher model the recursion relation is reduced to a one-dimensional integral equation which can be solved numerically giving $\nu = 0.652$ at $d = 3$, or by ϵ expansion in agreement with the results of Wilson and Fisher to leading order in ϵ. The method is also used to calculate thermodynamic functions for the $d = 2$ Ising model; excellent agreement with the Onsager solution is found.

KEY WORDS: Variational approximations; renormalization group eigenvalues; thermodynamic functions.

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1. METHODOLOGY

1.1. Renormalization Transforms

At the most elemental level, statistical mechanics is concerned with the calculation of a free energy F in terms of a sum over states or statistical configurations. This sum is defined by a Hamiltonian H, which depends upon some coordinates σ. The sum over states can be written as an integral or sum over a "phase space," $\int d\Gamma_\sigma$. Then the fundamental formula of statistical mechanics expresses the dependence of the free energy upon the Hamiltonian as

$$F_\sigma\{H\} = -\ln \int d\Gamma_\sigma \, e^{-H(\sigma)} \tag{1}$$

The subscript σ on the left-hand side of Eq. (1) indicates that F is defined as a sum over the σ-space. The remainder of statistical mechanics is concerned with the definition and evaluation of statistical averages. Formally, this can be achieved by expressing H in the form

$$H(\sigma) = H_0(\sigma) + \lambda V(\sigma) \tag{2a}$$

the averages are given by derivatives of the free energy, e.g.,

$$\langle V \rangle_\lambda = \partial F_\sigma\{H_\lambda\}/\partial\lambda \tag{2b}$$

$$\langle (V - \langle V \rangle_\lambda)^2 \rangle_\lambda = -\partial^2 F_\sigma\{H_\lambda\}/\partial\lambda^2 > 0 \tag{2c}$$

At the same level of generality, one can consider the renormalization group to be a set of transformations[1–5,2] from the old statistical variables σ to new variables μ and from the old Hamiltonians $H(\sigma)$ to new Hamiltonians $H'(\mu)$. In general we write this transformation as

$$H' = R\{H\} \tag{3}$$

We demand that these transformations leave the free energy invariant, i.e., that

$$F_\mu(R\{H\}) = F_\sigma\{H\} \tag{4}$$

where F_μ is defined as a sum over the new variables, i.e.,

$$F_\mu\{H'\} = -\ln \int d\Gamma_\mu \exp[-H'(\mu)] \tag{5}$$

The transformations (3) are most conveniently defined by constructing a set of functions of both μ and σ of the form[3,6]

$$\hat{H}(\mu, \sigma) = H(\sigma) - \hat{T}(\mu, \sigma) - U_{\hat{T}}(\sigma) \tag{6a}$$

[2] Reviews of the renormalization method are given in Refs. 1–5.

Here T is arbitrary, but U is defined by the relation

$$U_{\hat{T}}(\sigma) = F_{\mu}(-\hat{T}) = -\ln \int d\Gamma_{\mu} \exp[\hat{T}(\mu, \sigma)] \tag{6b}$$

In this paper, we use a caret to indicate functions (like $\hat{H}$ and $\hat{T}$) which depend upon both σ and μ.

To see the fundamental renormalization property, consider the sum over both sets of variables

$$\begin{aligned} F_{\mu\sigma}\{\hat{H}\} &= -\ln \int d\Gamma_{\mu}\, d\Gamma_{\sigma} \exp[-\hat{H}(\mu, \sigma)] \\ &= F_{\mu}\{F_{\sigma}\{\hat{H}\}\} = F_{\sigma}\{F_{\mu}\{\hat{H}\}\} \end{aligned} \tag{7}$$

The second line of (7) is an identity which holds for all $\hat{H}$. It simply expresses the fact that the sum over μ and σ can be calculated in either order. Now, specialize to the case in which $\hat{H}$ is defined by Eq. (6). Because of the definition of $U_{\hat{T}}$,

$$F_{\mu}\{\hat{H}\} = H(\sigma) \tag{8}$$

Hence, the right-hand side of (7) is the basic free energy. On the other hand, Eq. (7) also defines the free energy as $F_{\mu}\{H'\}$ with H' defined as

$$\begin{aligned} H'(\mu) &= F_{\sigma}\{H + U_{\hat{T}} - \hat{T}\} \\ &= -\ln \int d\Gamma_{\sigma} \exp[H(\sigma) + U_{\hat{T}}(\sigma) - \hat{T}(\mu, \sigma)] \end{aligned} \tag{9a}$$

Equation (9a) defines H' as a function of $\hat{T}$ and H. We define this dependence in a more compact notation by writing

$$R_{\hat{T}}\{H\} = F_{\sigma}\{H + U_{\hat{T}} - \hat{T}\} \tag{9b}$$

Equation (9a) or Eq. (9b) defines the renormalization operation that generates H' from H. Thus, Eq. (7) generates once more the fundamental invariance equation of the renormalization group

$$F_{\sigma}\{H\} = F_{\mu}\{R_{\hat{T}}\{H\}\} \tag{10}$$

while Eqs. (6) and (7) define a whole class of renormalization transformations.

1.2. Upper and Lower Bounds

In practical applications, one seeks to calculate $F_{\sigma}\{H\}$ by constructing approximations to $R_{\hat{T}}\{H\}$. After many successive transformations of this form, the Hamiltonian will either simplify to a tractable form or reach a "fixed point" which will have relatively simple qualitative properties.

However, in choosing approximations to $R_{\hat{T}}\{H\}$, one would like to have criteria for deciding whether one approximation is better than another. We suggest "variational" criteria.[3] That is, we suggest the construction of approximate renormalizations or recursions of the form $H' = R^L\{H\}$ and $H' = R^U\{H\}$. While the exact renormalizations leave the free energy unchanged, the approximate ones, R^U and R^L, do not. Rather, they are chosen to produce an error of known sign, i.e., they have the properties

$$F_\mu\{R^U\{H\}\} \geqslant F_\mu\{R_{\hat{T}}\{H\} = F_\sigma\{H\} \geqslant F_\mu\{R^L\{H\}\} \tag{11}$$

Imagine, then, that we have constructed a whole set of upper (lower) bound renormalizations R^U (R^L), which obey (11). Notice that if we apply many successive upper (lower) bound renormalizations, we get a composite relation which obeys the upper (lower) bound property. After many such recursions we have an approximate result for the free energy which is an upper (lower) bound to the true free energy.

However, at each step of recursion, we could have chosen any one of a large number of different approximate renormalizations by choosing different $\hat{T}$'s or by varying the other parameters which define the upper (lower) bound relations. Hopefully, one might obtain good results for physical quantities by choosing the upper (lower) bound recursions that give the smallest error in the free energy. Thus, we propose the construction of a minimum upper bound to the free energy.

We say "hopefully" because usually one is not interested in the free energy itself. Rather its derivatives are of the major physical interest. Since the variational principles pertain to the free energy, there is no guarantee that the derivatives will be accurate.

To obtain actual expressions for the bounding renormalizations, return to Eq. (7), rewritten in the form

$$F_\sigma\{H\} = F_{\mu\sigma}\{\hat{H}\} = F_\mu\{F_\sigma\{\hat{H}\}\} \tag{12}$$

In the exact calculation, $\hat{H}$ is given by Eq. (6). To generate approximations, we replace the exact $\hat{H}$ by $\hat{H}^A$ and generate an approximate H' as

$$H^A(\mu) = F_\sigma\{H^A\} = -\ln \int d\Gamma_\sigma \exp[-\hat{H}^A(\mu, \sigma)] \tag{13a}$$

Since $\hat{H}^A$ will depend upon H, we can say that Eq. (13a) defines an approximate recursion relation

$$H^A = R^A\{H\} \tag{13b}$$

[3] For a preliminary report on variational principles and approximate renormalization group calculations see Ref. 7.

Then this approximate renormalization will be an upper (lower) bound relation if

$$\Delta F = F_{\mu\sigma}\{\hat{H}\} - F_{\mu\sigma}\{\hat{H}^A\} \tag{14}$$

is less (greater) than or equal to zero.

Standard methods immediately generate criteria for $\hat{H}^A$'s that satisfy these conditions. Define an error, which is hoped to be small, by

$$\hat{V}(\mu, \sigma) = \hat{H}(\mu, \sigma) - \hat{H}^A(\mu, \sigma) \tag{15a}$$

and write

$$\hat{H}_\lambda = \hat{H}^A + \lambda\hat{V} \tag{15b}$$

The approximation is defined by $\hat{H}_{\lambda=0}$; the exact theory by $\hat{H}_{\lambda=1}$. In direct analogy with Eq. (2), we define

$$\langle\hat{V}\rangle_\lambda = \partial F_{\mu\sigma}\{\hat{H}_\lambda\}/\partial\lambda \tag{16}$$

$$E_\lambda = \langle(\hat{V} - \langle\hat{V}\rangle_\lambda)^2\rangle_\lambda = -(\partial^2/\partial\lambda^2)F_{\mu\sigma}\{\hat{H}_\lambda\} \tag{17}$$

Note that $E_\lambda > 0$. The errors will be proportional to E_λ.

It is easy to generate two identities for ΔF, namely

$$\Delta F = \langle\hat{V}\rangle_{\lambda=0} - \int_0^1 d\lambda\,(1 - \lambda)E_\lambda \tag{18a}$$

$$= \langle\hat{V}\rangle_{\lambda=1} + \int_0^1 d\lambda\,\lambda E_\lambda \tag{18b}$$

Our job is to fix the sign of ΔF. To get the two types of recursion, one chooses

$$\langle\hat{V}\rangle_{\lambda=0} = 0; \qquad \text{for the upper bound} \tag{19a}$$

$$\langle\hat{V}\rangle_{\lambda=1} = 0; \qquad \text{for the lower bound} \tag{19b}$$

1.3. Realization of Upper Bounds

The upper bound approximations are easily realized. Choose H^A to be of the form

$$\hat{H}^A(\mu, \sigma) = \psi(\mu, \sigma) + H_1(\mu) \tag{20}$$

Here ψ is a variational function which is simple enough so that one can calculate

$$H_0(\mu) = -\ln\int d\Gamma_\sigma\, e^{-\psi(\mu,\sigma)} = F_\sigma(\psi) \tag{21}$$

and averages of the form

$$\langle\hat{V}(\mu, \sigma)\rangle_\psi = \int d\Gamma_\sigma\, \hat{V}(\mu, \sigma)e^{-\psi(\mu,\sigma)+H_0(\mu)} \tag{22}$$

Condition (19a) reduces to

$$H_1(\mu) = \langle H(\sigma) - \hat{T}(\mu, \sigma) - U_{\hat{T}}(\sigma) - \psi(\mu, \sigma)\rangle_{\psi} \tag{23a}$$

which can be expressed symbolically by

$$H_1 = R_{\psi}{}^1(H - \hat{T} - U_{\hat{T}} - \psi) \tag{23b}$$

From Eq. (13a)

$$H^A(\mu) = H_0(\mu) + H_1(\mu)$$

Hence the upper bound recursion is

$$R^U\{H\} = F(\psi) + R_{\psi}{}^1(H - \hat{T} - U_{\hat{T}} - \psi) \tag{24}$$

Equation (23) expresses the extension of the standard variational principle of statistical mechanics[8] to renormalization calculations.

1.4. Symmetry Properties

Renormalization calculations are enormously simplified when the symmetries of the problem are properly taken into account. Let the problem in the σ-space be symmetric under transformations g_i, $i = 1, 2,...$, defined by

$$\sigma \to \sigma' = g_i(\sigma) \tag{25a}$$

while the problem in μ is symmetric under G_j, $j = 1, 2,...$, defined by

$$\mu \to \mu' = G_j(\mu) \tag{25b}$$

We say that Hamiltonians $H(\sigma)$ obey the symmetries if $H(g_i(\sigma)) = H(\sigma)$ and $d\Gamma_{g_i(\sigma)} = d\Gamma_{\sigma}$ for all i. A symmetric $H'(\mu)$ is defined in a similar manner. A major goal in the construction of renormalization calculations is to ensure that $H'(\mu)$ is properly symmetric whenever $H(\sigma)$ is symmetric.

As a specific example, the σ and μ variables might each be arranged on a lattice, so that they could be represented as $\sigma(r)$ and $\mu(R)$. Then the symmetries (25) would include lattice coordinate transformations of the form

$$\sigma' = g_i(\sigma)$$

whenever

$$\sigma'(r) = \sigma(\mathbf{g}_i(r)) \tag{26a}$$

and

$$\mu' = G_j(\mu)$$

whenever

$$\mu'(R) = \mu(\mathbf{G}_j(R)) \tag{26b}$$

Here, $\mathbf{g}_i$ and $\mathbf{G}_j$ describe all possible lattice translation and rotation operations.

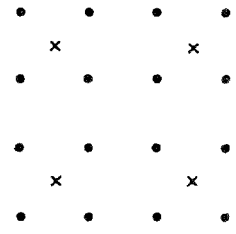

Fig. 1. The basic lattice. ● = σ and × = μ.

The general method of ensuring the symmetry of $H'(\mu)$ given that of $H(\sigma)$ is to embed the μ-lattice within the σ-lattice. One example of such a pair of lattices is shown in Fig. 1. In general, we shall want the μ variable to have fewer degrees of freedom than the σ variables so that the symmetry operations G_j are a subset of the operations g_j. In the case shown in Fig. 1, g_i includes all translations with a displacement $(n, m)a_0$ and integral n and m, while G_j requires n and m to be even integers.

Now assume that $H(\sigma)$ and $d\Gamma_\sigma$ are symmetric under all g_i while $d\Gamma_\mu$ is symmetric under all G_j. In the exact renormalization calculation, i.e., Eq. (8), the symmetry of $H(\sigma)$ will ensure the symmetry of $H'(\mu)$ whenever

$$\hat{T}(G_j(\mu), G_j(\sigma)) = \hat{T}(\mu, \sigma) \tag{27}$$

for all j. In the upper bound calculation, defined by Eq. (22), $H'(\mu)$ will be properly symmetric whenever $\psi(\mu, \sigma)$ obeys a relation like (26).

The symmetry conditions play an even more essential role in the construction of lower bound renormalizations. For it is only with the aid of these conditions that we can ensure that the average of $\hat{V}$ vanishes, as in Eq. (18b). Since this equation describes an average in the presence of the exact $\hat{H}$, this average cannot be calculated explicitly. But, if one makes $\hat{V}$ into a sum of terms, each odd under some symmetry operation, then Eq. (18b) will certainly be satisfied. With this end view, split $\hat{V}$ into two terms:

$$\hat{V}(\mu, \sigma) = \hat{V}_A(\mu, \sigma) + V_a(\sigma) \tag{28}$$

The subscripts indicate functions which are antisymmetric, with $\hat{V}_A$ being a sum of terms antisymmetric in at least one subgroup operation

$$\hat{V}_A(\mu, \sigma) = \sum_j V_{A,j}(\mu, \sigma)$$

with

$$V_{A,j}(G_j(\mu), G_j(\sigma)) = -V_{A,j}(\mu, \sigma) \tag{29}$$

On the other hand, $V_a(\sigma)$ is symmetric under all these operations

$$V_a(G_j(\sigma)) = V_a(\sigma) \qquad \text{for all } j \tag{30a}$$

but is a sum of terms each antisymmetric under one of the remaining g_i operations, i.e.,

$$V_a(\sigma) = \sum_i V_{a,i}(\sigma) \tag{30b}$$

with

$$V_{a,i}(g_i(\sigma)) = -V_{a,i}(\sigma) \tag{30c}$$

One can see immediately that Eq. (19b) is satisfied by this form of $\hat{V}$ if $H(\sigma)$ is symmetric under all g_i and if $\hat{T}$ obeys (27). To see this one need only write (19b) as

$$0 = \int d\Gamma_\mu \, d\Gamma_\sigma \{\exp[\hat{T}(\mu, \sigma) - U_{\hat{T}}(\sigma) - H(\sigma)]\} \sum_j \hat{V}_{A,j}(\mu, \sigma) + \int d\Gamma_\sigma \{\exp[-H(\sigma)]\} \sum_i V_{a,i}(\sigma) \tag{31}$$

Every term in the sum over i or j vanishes because of one or another of the symmetry operations.

Now that Eq. (19b) has been verified, one can rewrite (13a) as

$$H^L(\mu) = -\ln \int d\Gamma_\sigma \{\exp[\hat{T}(\mu, \sigma) - H(\sigma) - U_{\hat{T}}(\sigma)]\} \times \exp[+\hat{V}_A(\mu, \sigma) - V_a(\sigma)] \tag{32a}$$

Equation (32a) defines the Hamiltonian that is generated by the lower-bound renormalization calculation. In a somewhat more implicit notation, one can write a formula analogous to Eq. (8b), namely

$$H^L = R_{\hat{T}}\{H - \hat{V}_A - V_a\} = F_\sigma\{H - \hat{V}_A - V_a + U_{\hat{T}} - \hat{T}\} \tag{32b}$$

In the absence of $\hat{V}_A$, $H^L(\mu)$ is certainly symmetric under all the operations G_j. In the remainder of this paper, we shall not include any terms like $\hat{V}_A$. However, one should notice that since $\hat{V}_A$ can certainly include all kinds of antisymmetric terms depending only upon μ but not upon σ, it is relatively easy to adjust $\hat{V}_A$ so that it generates a fully symmetric H^L.

1.5. Renormalizations and Recursion Relations Near Fixed Points

In general, one may write any symmetric $H(\sigma)$ in the form

$$H(\sigma) = -\sum_i K_i S_i(\sigma) \tag{33}$$

Here the K_i form a vector $\mathbf{K}$ of coupling constants, while the $S_i(\sigma)$ are the complete set of functions of the σ that obey all the symmetries. We denote an H of the form (33) as $H_{\mathbf{K}}(\sigma)$. After the renormalization, an $H'(\mu)$ is generated, which obeys the same symmetries and is hence expressible as $H_{\mathbf{K}'}(\mu)$, where

$\mathbf{K}'$ is a new set of couplings. For this reason, the renormalization may be visualized as a recursion relation which expresses $\mathbf{K}'$ as a function of $\mathbf{K}$. This recursion relation is written

$$\mathbf{K}' = R_{\mathbf{t}}(\mathbf{K}) \tag{34}$$

Similarly, the approximate renormalizations may be expressed as

$$\mathbf{K}' = R_{\mathbf{p}}{}^{A}(\mathbf{K}) \tag{35}$$

where $\mathbf{p}$ includes the parameters in $\hat{T}$ as well as any other variational parameters.

The free energy $F_\sigma\{H_{\mathbf{K}}(\sigma)\}$ can be written as a product of the number of sites N and a free energy per site $f(\mathbf{K})$. If there are N' sites after the renormalization, the basic inequality (10) may be conveniently expressed as

$$f(R_{\mathbf{p}}{}^{U}(\mathbf{K})) \geqslant f(R_{\mathbf{t}}(\mathbf{K})) = (N/N')f(\mathbf{K}) \geqslant f(R_{\mathbf{p}}{}^{L}(\mathbf{K})) \tag{36}$$

The standard method of dealing with near-critical behavior starts from the calculation of an approximate fixed point $K_A{}^*(p)$, which obeys

$$K_A{}^*(p) = R_p{}^{A}(K_A{}^*(p)) \tag{37}$$

The next step is the calculation of the recursion relation near the fixed point by writing

$$b_{ij}^{A} = \frac{\partial}{\partial K_j}[R_{\mathbf{p}}{}^{A}(\mathbf{K})]_i \Big|_{\mathbf{K}=K_A{}^*(p)} \tag{38}$$

For later reference, we shall also need $W_{i,m}^{A}$, the derivative of the ith component of the recursion relation with respect to the mth parameter at fixed $\mathbf{K}$,

$$W_{i,m}^{A} = \frac{\partial}{\partial p_m}[R_p{}^{A}(K)]_i \Big|_{\mathbf{K}^*=K_A{}^*(p)} \tag{39}$$

Both W^A and b^A depend upon $\mathbf{p}$.

Physical information about the critical indices is obtained from the eigenvalues of b_{ij}^{A}.[9] Define eigenvalues $b_\alpha{}^A$ and left and right eigenvectors $v_{\alpha i}^{A}$, $u_{j\alpha}^{A}$ by

$$\sum_i v_{\alpha i}^{A} b_{ij}^{A} = b_\alpha{}^{A} v_{\alpha j}^{A}, \qquad \sum_i b_{ij}^{A} u_{j\alpha}^{A} = u_{i\alpha}^{A} b_\alpha{}^{A} \tag{39a}$$

For variational calculations, the most important eigenvalue is the trivial one

$$b_0{}^{A} = N/N' \tag{39b}$$

This trivial eigenvalue is generated by choosing $S_0(\sigma)$ to be just N. A change in the conjugate coupling constant K_0, i.e., ΔK_0, leads to a change in K_0', which is given by

$$(\Delta K_0')N' = (\Delta K_0)N$$

Hence b_{i0}^A is exactly $(N/N')\,\delta_{i,0}$. The corresponding right eigenstate is also trivial,

$$u_{i0}^A = \delta_{i0} \tag{39c}$$

but the left eigenstate v_{0i}^A must be calculated in detail. If this eigenstate is normalized by taking

$$v_{00}^A = 1 \tag{40}$$

Then v_{0i}^A has a very direct calculational significance: When $K_i = K_i^*(p) + h_i$ then, for very small h_i, the leading term in $f(\mathbf{K})$ is

$$f(\mathbf{K}_A^*(p) + \mathbf{h}) = \sum_i v_{0i}^A h_i + \text{higher order in } h \tag{41}$$

Hence v_{0i}^A is proportional to the average value of S_i at the fixed point:

$$v_{0i}^A(p) = (1/N)\langle S_i(\sigma)\rangle_{H_{K_A^*(p)}} \tag{42}$$

Equation (42) is equally true for the approximate or the exact calculations of the free energy.

These results provide a relatively simple variational technique for fixing $\mathbf{p}$. According to the variational scheme, the "best" value of $\mathbf{p}$ should have the property that the calculated free energy should be extremal with respect to variations of $\mathbf{p}$ at fixed $\mathbf{K}$. We demand this condition at K^*. According to Eq. (37), the change in K_i' when we hold K^* at $K_A^*(p)$ but vary p_m by the amount Δp_m is $W_{i,m}^A\,\Delta p_m$. The condition that this change produce no first-order variation in the free energy is, according to Eq. (41), the statement

$$\sum_i v_{0i}^A(p) W_{im}^A(p) = 0 \tag{43}$$

There are as many equations (43) as there are variational parameters p_m. These equations are then used to determine $\mathbf{p}$. Once $\mathbf{p}$ is determined, the critical indices are known.

2. AN EXAMPLE: THE ONE-HYPERCUBE APPROXIMATION

2.1. Derivation

There are many examples of usable upper bound renormalization approximations. All of the first-order perturbation expansions described by Neimeijer and van Leeuwen[4] as used by Hsu *et al.*[10] are upper limit approximations. These approximations, and others we have employed, do not give very good answers either in the critical region or elsewhere. On the other hand, one can find a class of lower bound renormalizations which give surprisingly good answers. In this section, we describe in a very general way how one can develop the simplest class of lower bound approximations.

Start from a set of spin variables $\sigma(\mathbf{r})$ defined at the points of a simple hypercubical lattice in d dimensions, i.e.,

$$r = (n_1 + \tfrac{1}{2}, n_2 + \tfrac{1}{2}, n_3 + \tfrac{1}{2}, \ldots, n_d + \tfrac{1}{2}) \tag{44}$$

for $n_1, n_2, \ldots$ integral. In this definition $\sigma(\mathbf{r})$ may be any statistical variable, which takes on continuous or discrete values. In addition, it may have all kinds of vector indices. The spins $\mu(\mathbf{R})$ are defined similarly on a hypercubical lattice of double the lattice constant in (44) i.e.,

$$R = 2(N_1, N_2, \ldots, N_d) \tag{45a}$$

for integral $N_1, N_2, \ldots$. Figure 1 illustrates this configuration for two dimensions.

To further describe the problem, we mentally divide the lattice into hypercubes centered at the ordinary lattice points $R = (n_1, n_2, \ldots, n_d)$, for all integral values of $n_1, n_2, \ldots$. Each of these hypercubes contains $z = 2^d$ vertices $\sigma(r)$, and each $\sigma(r)$ lies in z hypercubes. Two kinds of hypercube will be particularly distinguished in this work:

1. The "blue" hypercubes centered at

$$R_b = 2(N_1, N_2, \ldots, N_d) + (1, 1, 1, \ldots, 1) \tag{45b}$$

2. The "red" hypercubes centered at the points (45a). Each spin lies in one and only one red hypercube and also only one blue hypercube. When r lies in a particular red hypercube R, we write $r \in R$; and when it lies in the blue hypercube, we write $r \in \tilde{R}$.

We can now express a very general renormalization scheme by writing $\hat{T}(\mu, \sigma)$ as

$$\hat{T}(\mu, \sigma) = \sum_R a(\mu(R)) + \sum_R \sum_{r \in R} b(\mu(R), \sigma(r)) = \sum_R \hat{t}(\mu(R), \sigma) \tag{46}$$

where a and b are arbitrary real-valued functions. Then, the subtraction function $U_{\hat{T}}(\sigma)$, as defined by Eq. (6), is expressible in terms of functions $u(\boldsymbol{\sigma}_R)$, where $\boldsymbol{\sigma}_R$ is the set of z variables $\sigma(r)$ with $r \in R$. This expression is

$$U_{\hat{T}}(\sigma) = \sum_R u(\sigma_{\mathbf{R}}) \tag{47a}$$

with

$$u(\sigma_{\mathbf{R}}) = \ln \int d\mu \exp\left[a(\mu) + \sum_{\mathbf{r} \in \mathbf{R}} b(\mu, \sigma(\mathbf{r}))\right] \tag{47b}$$

Once these definitions are given, the exact renormalization transformation is

$$\exp[-H'(\mu)] = \int d\Gamma_0 \exp[-H(\sigma)] \times \exp\left\{\sum_{\mathbf{R}} \left[a(\mu(\mathbf{R})) - u(\sigma_R) + \sum_{\mathbf{r} \in \mathbf{R}} b(\mu(\mathbf{R}), \sigma(\mathbf{r}))\right]\right\} \tag{48}$$

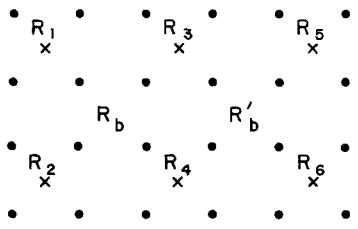

Fig. 2. R_1, R_2, R_3, R_4 satisfy $R_i \in R_b$; R_3, R_4, R_5, R_6 satisfy $R_i \in R_b'$.

while the lower bound approximation takes the form

$$\exp[-H^L(\mu)] = \int d\Gamma_\sigma \{\exp[-H(\sigma) - \hat{V}(\mu, \sigma)]\} \exp\left[\sum_R \hat{t}(\mu(\mathbf{R}), \sigma) - \mu(\sigma_\mathbf{R})\right] \tag{49}$$

In order that Eq. (49) define a lower bound approximation, we must choose $\hat{V}$ to obey Eq. (18b).

But before we define such a $\hat{V}(\mu, \sigma)$, let us choose a specific simple form of $H(\sigma)$. Let $\mathbf{R}'$ represent the centers of all hypercubes—red, blue, and the remainder (which we call green hypercubes). Let $\sigma_{\mathbf{R}'}$ be the set of all spins $\sigma(\mathbf{r})$ with $\mathbf{r} \in \mathbf{R}'$. Then take $H(\sigma)$ in the form

$$H(\sigma) = -\sum_{R'} v(\sigma_{\mathbf{R}'}) \tag{50a}$$

Write the integration as an integral over the variables in the different blue hypercubes

$$\int d\Gamma_\sigma = \prod_{\mathbf{R}_b} \int d\gamma_{\mathbf{R}_b}, \qquad d\gamma_{\mathbf{R}_b} = \prod_{\mathbf{r} \in \mathbf{R}_b} d\sigma(r) \tag{50b}$$

Next, define $\mathbf{R} \in \mathbf{R}_b$ whenever the red hypersphere centered at $\mathbf{R}$ touches the blue one centered at $\mathbf{R}_b$. This touching is shown in Fig. 2. Finally, note that each $\mathbf{R} \in \mathbf{R}_b$ uniquely defines a single point which satisfies both $\mathbf{r} \in \mathbf{R}$ and $r \in \mathbf{R}_b$ (see Fig. 3). We define this relationship by writing $\mathbf{r} \in (\mathbf{R}, \mathbf{R}_b)$. With all these definitions, Eq. (49) may be written in the form

$$\exp[-H^L(\mu)] = \int \left\{\prod_{\mathbf{R}_b} d\gamma_{\mathbf{R}_b} \exp[+\hat{v}(\sigma_{\mathbf{R}_b}, \mu_{\mathbf{R}_b})]\right\} \exp[-\hat{V}(\mu, \sigma) + V_a(\sigma)] \tag{51}$$

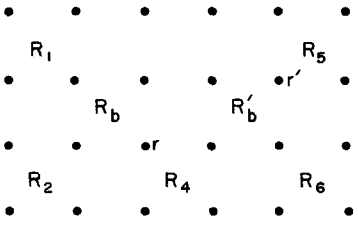

Fig. 3. $r \in (R_b, R_4)$; $r' \in (R_b', R_5)$.

with

$$v(\sigma_{R_b}, \mu_{R_b}) = \frac{1}{z} \sum_{\mathbf{R} \in \mathbf{R}_b} a(\mu(\mathbf{R})) + \sum_{R \in R_b} \sum_{r \in R_b, R} b(\sigma(\mathbf{r}), \mu(\mathbf{R})) + zv(\sigma_{\mathbf{R}_b}) - u(\sigma_{\mathbf{R}_b}) \tag{52a}$$

and

$$V_a(\sigma) = \sum_{R_b} u(\sigma_{\mathbf{R}_b}) - \sum_{R} u(\sigma_{\mathbf{R}}) + \sum_{R'} v(\sigma_{R'}) - z \sum_{R_b} v(\sigma_{R_b}) \tag{52b}$$

We are about to show that the $V_a(\sigma)$ defined by Eq. (52b) obeys all the conditions of (29). Once this demonstration is completed, we can simplify Eq. (51) by making the particular choice

$$\hat{V}(\mu, \sigma) = V_a(\sigma) \tag{53}$$

Then (51) gives H^L in terms of a product of integrals which are all independent of one another. Thus, (51) implies that

$$H^L(\mu) = \sum_{\mathbf{R}_b} v'(\mu_{\mathbf{R}_b}) \tag{54}$$

That is, the new H has exactly the same form (50a) as the old H. Then our approximate recursion relation becomes

$$\exp[\hat{v}'(\mu_{\mathbf{R}_b})] = \int d\gamma_{\mathbf{R}_b} \exp[\hat{v}(\sigma_{\mathbf{R}_b}, \mu_{\mathbf{R}_b})] \tag{55}$$

The proof that $V_a(\sigma)$ obeys (29) is very simple and direct. The symmetry operations G_j are composed of translations through two lattice constants

$$r \to r + (2, 0, 0, \ldots)$$

and rotation through 90° about each cubic axis. All four terms in (52b) are symmetric under each G_j. Hence (29) follows immediately. Next note that the first two terms in (52b) are antisymmetric under the transformation red $\leftrightarrow$ blue, i.e.,

$$r \to r + (1, 1, 1, \ldots)$$

Hence, these terms obey all of Eq. (29). Finally, the last two terms in (52b) may be written as

$$\sum_{R_i} \sum_{R_b} [v(\sigma_{\mathbf{R}_b + \mathbf{r}_i}) - v(\sigma_{\mathbf{R}_b})] \tag{56}$$

Here r_i are all the $z = 2^d$ different lattice vectors,

$$r_i = (n_1, n_2, \ldots, n_d)$$

with each n taking on the values 0 and 1. Thus (56) is a sum of terms each antisymmetric under the transformation

$$r \to -r - r_i$$

plus the parity operation. QED

2.2. Specification of the Approximation

Equation (55) may be simplified if we consider that the $\mu(\mathbf{R})$ for $\mathbf{R} \in \mathbf{R}_b$ are numbered in some manner $\mu(\mathbf{R}) \to \mu_i$ for $i = 1, 2, 3, \ldots, z = 2^d$. Corresponding to each μ_i there is a single σ_i. Then, Eq. (55) reduces to

$$\exp[v'(\mu)] = \int d\sigma_1 \cdots d\sigma_z \exp[\hat{v}(\sigma, \mu)] \tag{57}$$

with (52a) implying

$$\hat{v}(\sigma, \mu) = \frac{1}{z} \sum_i a(\mu_i) + \sum_i b(\mu_i, \sigma_i) + zv(\sigma) - u(\sigma) \tag{58}$$

and (47b) implying

$$u(\sigma) = \ln \int d\mu \exp\left[a(\mu) + \sum_i b(\mu, \sigma_i)\right] \tag{59}$$

Each μ_i or σ_i may be a composite variable with many internal indices. The "integrals" in (57) and (59) may be really only sums over a finite set of possible values. Eqs. (57)–(59) represent our basic approximation—the simplest general case of a lower bound recursion approximation.

2.3. Case I: The Ising Model

In this case each σ_i and μ_i takes on two possible values, ± 1. The most general form of $a(\mu)$ is $p_0\mu$, and the most general form of $b(\mu, \sigma)$ is $p_1(\mu\sigma)$, where p_0 and p_1 are two parameters which define the transformation. Equation (59) then gives

$$u(\sigma) = u(s_1) = \ln 2 \cosh[p_0 + p_1 s_1(\sigma)] \tag{60}$$

with

$$s_1(\sigma) = \sum_{i=1}^{z} \sigma_i \tag{61}$$

Equation (57) then reduces to

$$\exp[v'(\mu)] = \sum_{\sigma_1 \ldots \sigma_z} \exp\left(\frac{1}{z} p_0 m_1 + p_1 \sum_i \sigma_i \mu_i\right) \exp[zv(\sigma) - u(s_1)] \tag{62}$$

with

$$m_1 = \sum_i \mu_i \tag{63}$$

In general $v(\sigma)$ may be expanded in terms of interaction constants. The first two terms are v_0 and $v_1 s_1$, where s_1 is the total magnetization in the hypercube. The next term is of the form

$$\sum_{i<j} v(|r_1 - r_j|)\sigma_i\sigma_j$$

Hence, the nearest-neighbor coupling may differ from the next-neighbor, etc. However, we may choose to deal with $v(\sigma)$, which obeys the symmetry condition that it is symmetric under the interchange of any two σ's, e.g.,

$$v(\sigma_1, \sigma_2, \sigma_3, \ldots, \sigma_3) = v(\sigma_2, \sigma_1, \sigma_3, \ldots, \sigma_3)$$

If $v(\boldsymbol{\sigma})$ obeys this permutation group symmetry, so will $v'(\mu)$. Let us assume this symmetry. Then $v(\sigma)$ will be of the form $v(s_1)$ and $v'(\mu)$ will be $v'(m_1)$. Thus, Eq. (62) reduces to

$$\exp[v'(m_1)] = \sum_{\sigma_1 \ldots \sigma_z} \exp\left[p_0 m_1/z + p_1 \sum_i \mu_i\sigma_i + zv(s_1) - u(s_1)\right] \tag{64}$$

The sum over the σ's is most conveniently represented in terms of the basic invariants of the permutation group $s_n(\sigma)$. There are $z + 1$ of these functions of the z spins σ_i. They are defined by setting $s_n(\sigma)$ equal to the sum of all products of r different σ's. Each of these is only a function of the s_1 defined by Eq. (61). More explicitly, we have

$$\begin{aligned} s_0 &= 1 \\ s_1 &= z, z-2, z-4, \ldots, -z \\ s_{n+1}(s_1) &= [s_1 s_n(s_1) - (z - n + 1)s_{n-1}]/(n+1) \end{aligned} \tag{65}$$

They obey the orthonormality condition

$$\sum_\sigma s_n(s_1)s_m(s_1) = \sum_{s_1} w(s_1)s_n(s_1)s_m(s_1) = \delta_{m,n}s_n(z)2^z \tag{66}$$

where the weight is given by

$$w(s_1) = \frac{z!}{[(z - s_1)/2]!\,[(z + s_1)/2]!} \tag{67}$$

With the aid of these definitions, after some arithmetic, we can reduce Eq. (64) to the form

$$\exp[v'(m_1)] = \sum_n \frac{s_n(m_1)}{s_n(z)} (\cosh p_1)^z (\tanh p_1)^n \left(\exp \frac{p_0 m_1}{z}\right) \Lambda_n \tag{68a}$$

with

$$\Lambda_n = \sum_{s_1} w(s_1)s_n(s_1) \exp[zv(s_1) - u(s_1)] \tag{68b}$$

$$u(s_1) = \ln 2 \cosh(p_0 + p_1 s_1) \tag{68c}$$

Thus, in d dimensions, a full recursion involves the calculation of $z + 2$ summations, each involving $z + 1$ terms.

2.4. Case II: A Generalized Gaussian Model

A very similar analysis may be applied to a generalized Gaussian model in which each $\sigma(r)$ is a vector with n components, written as $\boldsymbol{\sigma}(\mathbf{r})$ or $\sigma_i(\mathbf{r})$, $i = 1, 2, \ldots, n$. Following Bell and Wilson,[11] we choose

$$\begin{aligned} a(\boldsymbol{\mu}(\mathbf{R})) &= -\frac{1}{2} a \sum_j \mu_j^2(\mathbf{R}) \\ b(\boldsymbol{\mu}(\mathbf{R}), \boldsymbol{\sigma}(\mathbf{r})) &= ab \sum_j \mu_j(\mathbf{R}) \sigma_j(\mathbf{r}) \end{aligned} \tag{69}$$

where a and b are adjustable parameters. Then, Eq. (47b) implies

$$u(\sigma_{\mathbf{R}}) = \frac{n}{2} \ln \frac{2\pi}{a} + \frac{ab^2}{2} \sum_j s_j(\mathbf{R}) \cdot s_j(\mathbf{R}) \tag{70}$$

with s_j the total spin on the hypercube

$$s_j(\mathbf{R}) = \sum_{\mathbf{r} \in R} \sigma_j(\mathbf{r}) \tag{71}$$

We then choose $H(\sigma)$ in form (50a) and further specialize $v(\sigma_{\mathbf{R}'})$ to be of the form

$$v(\sigma_{\mathbf{R}'}) = -(1/2z) \sum_{\substack{\mathbf{r} \in R' \\ j}} \sigma_j^2(\mathbf{r}) + V(\mathbf{s}(\mathbf{R}')) \tag{72}$$

Thus, v involves an arbitrary function V of the total magnetization on the hypercube in addition to the trivial Gaussian term. The factor $1/z$ in Eq. (72) is designed to make the coefficient of $\sigma_i^2(r)$ in $H(\sigma)$ exactly 1/2. This choice essentially normalizes the Gaussian variables. Now, Eqs. (52) and (55) reduce to

$$\begin{aligned} &\exp\left[v'(m(\mathbf{R}_b)) - \frac{1}{2z} \sum_{\mathbf{R} \in \mathbf{R}_b} \sum_j \mu_j^2(\mathbf{R}_b)\right] \\ &\quad = \int \left\{ \prod_j \prod_{\mathbf{r} \in \mathbf{R}_b} d\sigma_j(r) \exp\left[-\frac{1}{2} \sigma_j^2(r)\right] \right\} \\ &\qquad \times \exp\left[zv(s(\mathbf{R}_b)) - \frac{1}{2} ab^2 s(\mathbf{R}_b) \cdot s(\mathbf{R}_b)\right] \\ &\qquad \times \exp\left[-\frac{1}{2z} a \sum_{\mathbf{R} \in \mathbf{R}_b} \sum_j \mu_j^2(R_b) - \frac{n}{2} \ln \frac{2\pi}{a}\right] \\ &\qquad \times \exp\left[b \sum_j \sum_{\mathbf{R} \in \mathbf{R}_b} \sum_{\mathbf{r} \in \mathbf{R}_b, \mathbf{R}} \mu_j(\mathbf{R}) \cdot \sigma_j(\mathbf{r})\right] \end{aligned} \tag{73}$$

Here $\mathbf{m}$ is the total cell magnetization, defined in exact analogy to Eq. (71),

$$\mathbf{m}(R_b) = \sum_{R \in R_b} \mu(R) \tag{74}$$

Equation (73) involves $z \times n$ integrals. If one fixes the n variables $s_j(R_b)$, the remaining $(n-1) \times z$ integrals are essentially trivial Gaussian integrals. After they are performed, Eq. (73) reduces to

$$\begin{aligned}
&\exp\left[v'(m) - \frac{1}{2z} \sum_{\mathbf{R} \in \mathbf{R}_b} \boldsymbol{\mu}(\mathbf{R}_b) \cdot \boldsymbol{\mu}(\mathbf{R}_b)\right] \\
&\quad = \exp\left[-\frac{1}{2z} \sum_{\mathbf{R} \in \mathbf{R}_b} \mu(R_b) \cdot \mu(R_b)[a - a^2 b^2 z] + \frac{nz}{2} \ln 2\pi\right] \\
&\qquad \times \int \frac{ds_1}{(2\pi z)^{1/2}} \cdots \frac{ds_n}{(2\pi z)^{1/2}} \exp\left[zv(\mathbf{s}) - \frac{1}{2} ab^2 \mathbf{s} \cdot \mathbf{s}\right] \\
&\qquad \times \exp\left(-\frac{a^2 b^2}{2z} \mathbf{m} \cdot \mathbf{m}\right) \exp\left[ab \frac{\mathbf{m} \cdot \mathbf{s}}{z} - \frac{n}{2} \ln \frac{2\pi}{a} - \frac{1}{2z} \mathbf{s} \cdot \mathbf{s}\right]
\end{aligned} \tag{75}$$

Equation (74) will hold if and only if the two kinds of terms on the right-hand side, i.e., those in $\mu \cdot \mu$ and those in $\mathbf{m} \cdot \mathbf{m}$, match the two terms on the left. The equality of the $\mu \cdot \mu$ terms implies

$$1 = a - a^2 b^2 z \tag{76}$$

while the equality of the other terms gives

$$\begin{aligned}
v'(m) = &-\frac{a^2 b^2}{2z} \mathbf{m} \cdot \mathbf{m} + \frac{n(z-1)}{2} \ln 2\pi - \frac{n}{2} \ln \frac{1}{a} + \ln \int \frac{ds_1}{(2\pi z)^{1/2}} \cdots \frac{ds_n}{(2\pi z)^{1/2}} \\
&\times \exp\left[zv(\mathbf{s}) - \frac{1}{2z} \mathbf{s} \cdot \mathbf{s}(1 + ab^2 z) + \frac{ab}{z} \mathbf{m} \cdot \mathbf{s}\right]
\end{aligned} \tag{77}$$

It is convenient to rewrite (78) and (79) in terms of the adjustable parameter

$$p = ab^2 z \tag{78}$$

so that (76) becomes

$$1/a = 1 - p \tag{79}$$

and (77) reads

$$\begin{aligned}
v'(m) = &-\frac{q^2}{2} \mathbf{m} \cdot \mathbf{m} + \frac{n(z-1)}{2} \ln 2\pi - \frac{n}{2} \ln(1-p) \\
&+ \ln \int \prod_j \frac{ds_j}{(2\pi z)^{1/2}} \exp\left[zv(s) - \frac{1}{2z} \mathbf{s} \cdot \mathbf{s}(1+p) + \frac{qm \cdot \mathbf{s}}{z^{1/2}}\right]
\end{aligned} \tag{80}$$

with

$$q = ab/z = [p/(1-p)]^{1/2}/z \tag{81}$$

3. GENERALIZED GAUSSIAN MODEL

In this section we discuss two special cases in which the recursion relation (80) can be solved analytically. We also discuss the results of a numerical solution of the one-dimensional integral Eq. (80).

3.1. The Gaussian Model $v(s) = v_0 + v_2(s^2)$

In this case the integral can be carried out exactly and we find

$$v_0' = zv_0 + \tfrac{1}{2}n[(z-1)\ln 2\pi - \ln(1-p) - \ln(p+1-K_2)] \quad (82)$$

and

$$K_2' = [p/(1-p)](M-1) \quad (83)$$

Here

$$M^{-1} = (1 - K_2 + p) \quad (84)$$

and

$$K_2 = 2z^2 v_2 \quad (85)$$

At the fixed point

$$K_2' = K_2 = K_2^* \quad (86)$$

Equations (83) and (84) are solved to give

$$K_2^* = 1 \quad (87)$$

It is easy to see that Eq. (82) is extremal at $p = \frac{1}{2}$, which is indeed a minimum of v_0.

The temperature eigenvalue is found by linearizing about the fixed point

$$\frac{\partial K_2'}{\partial K_2} = M^2\left(\frac{p}{1-p}\right)\Big|_{p=1/2} = 4 \quad (88)$$

In the usual notation[9] we have then

$$2^{y_\epsilon} = 4 \Rightarrow y_\epsilon = 2 \Rightarrow \nu = \tfrac{1}{2} \quad (89)$$

The magnetic eigenvalue is obtained by noticing that

$$bz = 2^{(d-2+\eta)/2} \quad (90)$$

As

$$bz = [zp(1-p)]^{1/2}|_{p=1,2} = 2 \quad (91)$$

we see that

$$\eta = 0 \quad (92)$$

Equations (89) and (92) are of course the expected values of the eigenvalues for the Gaussian model.

3.2. The Wilson–Fisher Model, ϵ Expansion[12]

In this case the generalized potential has the form

$$v(s) = v_0 + v_2 s^2 + v_4 s^4 + v_6 s^6 + \cdots \tag{93}$$

$$s^{2n} = (s^2)^n \tag{94}$$

and Eq. (80) becomes

$$v'(\mathbf{m}) = -\frac{1}{2z^2}\frac{p}{1-p}\,\mathbf{m}\cdot\mathbf{m} + \frac{n(z-1)}{2}\ln 2\pi + \frac{n}{2}\ln(1-p) + \ln I \tag{95}$$

where

$$\ln I = \ln \prod_i \int \frac{ds_i}{(2\pi)^{1/2}} \exp\left[-M^{-1}s^2 + q\frac{m_1 s_1}{z} + z^3 v_4 s^4 + z^4 v_6 s^6 + \cdots\right] \tag{96}$$

we have chosen

$$m = (m_1, 0, 0, 0, \ldots) \tag{97}$$

and performed a simple change of variable $s_i' = s_i/\sqrt{z}$. As we will see, in $4-\epsilon$ dimensions, $v_4 \sim \epsilon$, $v_6 \sim \epsilon^2, \ldots$. Anticipating this, we expand Eq. (96) in powers, of ϵ, keeping consistently all terms to a given order in ϵ. We find

$$\ln I = \ln I_0 + K_4 z^3 \langle s^4\rangle + K_6 z^4 \langle s^6\rangle + \frac{(K_4 z^3)^2}{2!}(\langle s^8\rangle - \langle s^4\rangle^2) + \cdots \tag{98}$$

here

$$\begin{aligned}\langle s^{2n}\rangle = &\left\{\int \frac{ds_1}{(2\pi)^{1/2}} \prod_{i=1}\int \frac{ds_i}{(2\pi)^{1/2}}\, s^{2n} \exp\left[-\frac{M^{-1}}{2}\left(s_1 - q\frac{Mm_1}{z}\right)^2\right]\right.\\ &\left.\times \exp\left(-\frac{M^{-1}}{2}s_i^2\right)\right\} \Big/ \left\{\int \frac{ds_1}{(2\pi)^{1/2}} \prod_{i=1}\int \frac{ds_i}{(2\pi)^{1/2}}\right.\\ &\left.\times \exp\left[-\frac{M^{-1}}{2}\left(s_1 - q\frac{Mm_1}{z}\right)^2\right] \exp\left(-\frac{M^{-1}}{2}s_i^2\right)\right\}^{-1}\end{aligned} \tag{99}$$

Some useful averages are

$$\langle s_1\rangle = qMm_1/z \tag{100}$$

$$\langle s_1^2\rangle - \langle s_1\rangle^2 = \langle s_2^2\rangle = \cdots = M \tag{101a}$$

$$\langle s_1^4\rangle = \langle s_1\rangle^4 + 6M\langle s_1^2\rangle + 3M^2 \tag{101b}$$

$$\langle s_2^4\rangle = 3M^2 \tag{101c}$$

Notice also that

$$\langle s^4 \rangle = \langle {s_1}^4 + 2(n-1){s_1}^2{s_2}^2 + (n-1){s_2}^4 + (n-1)(n-2){s_2}^2{s_3}^2 \rangle \quad (102)$$

Carrying out the integral and using the averages defined above, we find the recursion relation

$$v_0' = \tfrac{1}{2}n[(z-1)\ln 2\pi + \ln(1-p)] + zv_0 + \tfrac{1}{2}n \ln M + v_4 z^3 M^2 n(n+2) \quad (103a)$$

$$K_2' = p(1-p)(M-1) + 4(n+2)v_4 z^3 (Mq)^2 M z^2 + \cdots \quad (103b)$$

$$v_4' = v_4 z^3 (Mq)^4 + \frac{(v_4 z^3)^2}{2!}(Mq)^4 M^2 8(5n+6) + (3n+12)(v_6 z^4)(Mq)^4 M + \cdots \quad (103c)$$

$$v_6' = v_6 z^4 (Mq)^6 + 16\frac{(v_4 z^3)^2}{2!}(Mq)^6 M + \cdots \quad (103d)$$

It is now straightforward to obtain the fixed point to order ϵ. First from Eq. (103d)

$$v_6^* = \tfrac{1}{6}(v_4^* z)^2 M z \quad (104)$$

demonstrating that $v_6^* \sim \epsilon^2$. Substituting Eq. (104) into (103c) and keeping only terms of first order in ϵ, we find

$$[1 - z^3(Mq)^4] = v_4^* z^4 [7n + 24] \quad (105)$$

If we recall that to leading order $(Mq)^4 = \frac{1}{16}$, it is easy to see that the left-hand side of the equation is at least of order ϵ. Explicit calculation shows that

$$\epsilon \ln 2 + 8(\delta K_2^*) + [7n + 24] z^4 v_4^* = 0 \quad (106)$$

where δK_2^* is the change in K_2^* from its Gaussian value. The reader will notice that there is also in principle a contribution to Eq. (106) from the change in the variational parameter p; this effect is, however, identically zero to leading order in ϵ. From Eqs. (103a)–(103d) again keeping only the leading order terms, we find

$$\delta K_2^* + \tfrac{2}{3}(n+2) v_4^* z^4 = 0 \quad (107)$$

Introducing

$$K_4^* = z^3 v_4^* 2(n+2) \quad (108)$$

we have

$$\epsilon \ln 2 + 8(\delta K_2^*) + \frac{7n+24}{2(n+2)} K_4^* z = 0 \quad (109)$$

and

$$\delta K_2^* + \tfrac{1}{3} K_4^* z = 0 \quad (110)$$

Hence at the fixed point

$$K_4{}^*z = -\epsilon \ln 2 \frac{6}{5} \frac{n+2}{n+8} \tag{111}$$

and

$$\delta K_2{}^* = \epsilon \ln 2 \frac{2}{5} \frac{n+2}{n+8} \tag{112}$$

As before we can find the temperature eigenvalue by varying Eqs. (103a)–(103d) around the fixed point

$$\begin{aligned} \delta K_2{}' &= [4(1 + 4\,\delta K_2{}^*) + 6zK_4{}^*]\,\delta K_2 + z\,\delta K_4 \\ &= [4 + (2/3)zK_4{}^*]\,\delta K_2 + z\,\delta K_4 \end{aligned} \tag{113}$$

and

$$\delta K_4{}' = 8K_4{}^*\,\delta K_2 + \delta K_4[1 + O(\epsilon)] \tag{114}$$

In principle there is a contribution to $\delta K_2{}'$ from the change in the variational parameter; however, once again this effect does not contribute at leading order in ϵ. The temperature eigenvalue is found from Eqs. (113) and (114) to be

$$\nu = \frac{1}{2} + \frac{1}{4} \frac{n+2}{n+8} \epsilon \tag{115}$$

in agreement with the calculations of Wilson and Fisher.[12]

In order to obtain the magnetic eigenvalue, we must find the leading correction to $b = [zp(1-p)]^{1/2}$, that is, we must find the leading order correction to the variational parameter p. The lowest left-hand eigenstate of the derivative matrix $\tilde{\tilde{b}}^A$ is

$$\mathbf{v}^0 = (1, n/12, \ldots) \tag{116}$$

Differentiating Eqs. (116) with respect to the parameter p, we find that the derivative of the transformation is, to lowest order in ϵ,

$$\mathbf{w}^0 = \left(\frac{n}{2} \left(\frac{1}{1-\lambda} - \frac{1}{\lambda} \right) - 2n(\delta K_2{}^*) - K_4 \frac{z}{2} n,\ -2K_4 z,\ 0, \ldots \right) \tag{117}$$

Hence the variational condition, Eq. (43), becomes

$$0 = v^0 \cdot w^0 = \frac{n}{2} \left(\frac{1}{1-\lambda} - \frac{1}{\lambda} \right) - 2n(\delta K_2{}^*) - 2K_4 \frac{z}{3} n \tag{118}$$

which determines λ. Making use of Eq. (110), we find that the change in the parameter λ is at least of order ϵ^2, which in turn implies that the magnetic eigenvalue

$$\eta = 0 \tag{119}$$

to order (ϵ^2).

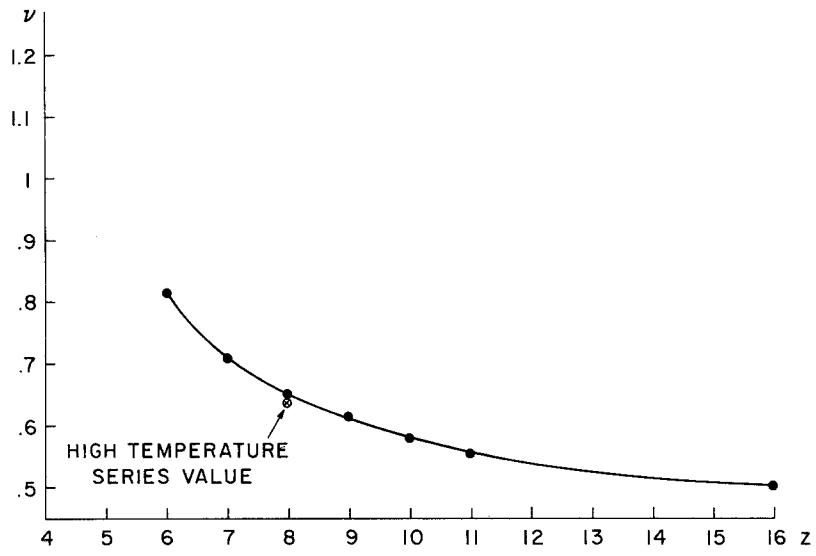

Fig. 4. The critical index ν as obtained from Eq. (80).

We see then that the approximation employed above is in fact an $\eta = 0$ approximation, although in coordinate space, it is similar in spirit to Wilson's[13] original work.

3.3. "Exact" Calculations

Finally we note that the recursion relation for the one-hypercube approximation to the Wilson–Fisher model is easily solved numerically. Equation (80) is simply a one-dimensional integral equation. It is solved for the fixed point v^*; then the parameter is adjusted as explained above. This adjustment gives the critical index δ or η. Unfortunately, it always gives $\eta < 0$. The error is not too bad since $\eta = -6 \times 10^{-4}$ at $z = 8$. Linearization of the equation about the fixed point gives the temperature eigenvalue from which the critical index ν can be obtained. In Fig. 4 we plot ν as a function of $z = 2^d$. The value of ν obtained for $d = 3$ is 0.6502, compared to the high-temperature series value of 0.642.[14] The eigenvalue grows unphysically large for $z < 5$.

4. ISING MODEL SOLUTION

Now, we return to Eqs. (68a)–(68c), which give the one-hypercube approximation for the Ising model. Once the s_r are calculated via Eq. (65),

Eqs. (68a)–(68c) give each iteration as a simple summation. The potential may be represented by writing

$$v(s_1) = \sum_i K_i s_i(s_1) \tag{120}$$

Note that in this representation, the Hamiltonian contains a constant term $-K_0 zN$ and a dimensionless magnetic field equal to zK_1. The standard nearest-neighbor and next-nearest-neighbor coupling constants are given by

$$K_{\text{nn}} = \tfrac{1}{2} zK_2, \qquad K_{\text{nnn}} = \tfrac{1}{4} zK_2 \tag{121}$$

To maintain the symmetry between spin up and spin down, we choose $p_0 = 0$. Since p_1 is the only remaining variational parameter, we simplify the notation by writing $p_1 = p$.

Thus, we can express Eqs. (68a)–(68c) in the form of recursion relations

$$K' = R^L(p, \mathbf{K}) \tag{122}$$

4.1. Fixed Points and Critical Indices

In two, three, and four dimensions there exists a range of p for which Eqs. (68a)–(68c) have at least three fixed points:

(a) A "strong coupling," stable fixed point with relatively large v_2.
(b) An unstable, "critical" fixed point with smaller v_2.
(c) A "weak coupling," stable fixed point with even smaller v_2.

We identify the critical point with the second type of fixed point.

The calculation proceeds by finding this fixed point for a particular value of p, i.e., finding $K_L^*(p)$, which obeys

$$K_L^*(p) = R^L(p, K_L^*(p)) \tag{123}$$

Then, $b_{ij}(r)$ is calculated as in Eq. (36), $W_i(p)$ as in Eq. (37), and $v_{0L}(p)$ as in Eq. (38). Here the subscript 0 refers to the trivial eigenstate with eigenvalue $z = 2^d$. Then the value of p is adjusted so that the extremum condition (43) is satisfied. This "best" value of p is described as p^*. This value of p and the corresponding nonzero coupling constants $K_i^*(p^*)$ are listed in Table I.

Next, the eigenvalues of b_{ij} are computed. Note that these computations of eigenvalues essentially describe situations in which p is held fixed during all recursions. That is, p is taken to be independent of the coupling constants. We shall see below that this is not a fully satisfactory approach. Table II lists the critical indices obtained from the two largest nontrivial eigenvalues. The eigenvalues are expressed in terms of the standard critical indices δ and α by writing

$$d/(2 - \alpha) = \ln_2 b', \qquad d/(1 + 1/\delta) = \ln_2 b' \tag{124}$$

Table I. Fixed Points for the One-Hypercube Approximation

Dimensionality d		2	3	4
Parameter value p^*		0.76598	0.40343	0.24992
Coupling constants	v_0	-0.88720	-0.73696	-0.70774
	v_2	0.13972	0.02097	4.0968×10^{-3}
	v_4	-0.006865	1.96×10^{-4}	3.23×10^{-5}
	v_6	—	-7.69×10^{-5}	-8.87×10^{-7}
	v_8	—	2.15×10^{-5}	-2.51×10^{-9}
	v_{10}	—	—	4.02×10^{-9}
	v_{12}	—	—	-3.91×10^{-10}
	v_{14}	—	—	-5.32×10^{-11}
	v_{16}	—	—	3.05×10^{-11}

Table II. Critical Indices as Derived from the One-Hypercube Approximation[a]

	Dimensionality d		
Critical index	2	3	4
δ	15.040	4.818	2.90
	(15)	(5.0 ± 0.2)	(3)
α	0.0017	0.1132	0.035
	(0)	(0.08 ± 0.04)	(0)
γ	1.7491	1.238	0.958
	(1.75)	(1.250 ± 0.005)	(1.0)
β	0.12457	0.3243	0.5033
	(0.125)	(0.3125 ± 0.005)	(0.5)
η	0.24937	0.0313	0.050
	(0.25)	(0.04 ± 0.03)	(0)
ν	0.9991	0.6289	0.491
	(1)	(0.639)	(0.5)

[a] For comparison, we list in parentheses values derived from other methods. For $d = 2$ and $d = 4$, the comparison values are exact; for $d = 3$ the comparison values are obtained from series expansions. In the latter case, the comparison values shown and particularly the errors indicated are all based to some extent upon the judgement of the authors. The index values other than δ and α shown as the result of our calculations are derived from scaling relations.

respectively for the first nontrivial even and odd spin eigenstates. The agreement with the exact results is surprisingly good at $d = 2$ and even reasonably good at $d = 4$. At $d = 3$, it is not clear whether the results listed are an improvement or a regression from the standard results of series calculations.

4.2. Free Energy Calculations

In the remainder of this section, we use the one-square approximation to calculate thermodynamic functions for the two-dimensional Ising model so that these may be compared with the Onsager solution.[4] This calculation involves three different types of recursions.

1. In a zeroth step of calculation, we perform a "decimation," i.e., a recursion[6] which is a sum over every other spin in the lattice, holding the remaining spins fixed. This recursion can be calculated exactly if the original Hamiltonian contains only a magnetic field h and a nearest-neighbor coupling K_{nn}. The result of this calculation is a potential on each new square of the form

$$v^1(s_1) = hs_1/4 + \ln 2 \cosh(h + K_{nn}s_1) \tag{125}$$

If the original lattice constant is 1, the new lattice constant is

$$a_1 = \sqrt{2} \tag{126}$$

2. Then, starting from the Hamiltonian defined by $v^1(s_1)$, the lower bound recursion is applied NI times, with variational parameters $p_1, p_2, \ldots, p_\alpha, \ldots, p_{NI}$. This calculation generates successively potential functions $v^2(s_1), \ldots, v^\alpha(s_1), \ldots, v^{1+NI}(s_1)$. After this is all done, the lattice constant is

$$a_{NI+1} = \sqrt{2} \times 2^{NI} \tag{127}$$

3. Finally, v^{1+NI} is used to generate an explicit expression for the free energy via a formula which permits the calculation of a rough lower bound to the free energy. To get this lower bound, the entropy is given its maximum possible value. If there are $\hat{N}$ sites on the lattice, this upper bound to the entropy is

$$\hat{S}/K = \hat{N} \ln 2 \tag{128}$$

Moreover, the energy is given its minimum possible value, obtained by writing

$$v(s_1) = \sum_i K_i s_i(s_1) \leqslant \sum_i |K_i| s_i(z) \tag{129}$$

[4] Thermodynamic functions for the two-dimensional Ising model have since been calculated by Nienhuis and Nauenberg.[16]

In total this lower bound to the free energy is given by

$$-F \leqslant \hat{N}\left[\ln 2 + \sum_{i>0} |K_i| s_i(z) + K_0\right] \tag{130}$$

since there is one square for each site in the lattice. In summary, if we have a Hamiltonian of the form (120), the free energy per site $f(\mathbf{K})$ is bounded by

$$-f(\mathbf{K}) \leqslant -f_0^L(\mathbf{K}) = \ln 2 + \sum_{i>0} |K_i| s_i(z) + K_0 \tag{131}$$

If the iterations successively generate interactions $\mathbf{K}^1, \mathbf{K}^2, \ldots, \mathbf{K}^\alpha, \ldots, \mathbf{K}^{NI+1}$, then Eq. (131) successively generates bounds on the free energy per site of the original problem, $f(K_{\text{nn}}, h)$, which are

$$-f(K_{\text{nn}}, h) \leqslant -(1/a_\alpha^2) f_0^L(\mathbf{K}^\alpha) - (1/a_\alpha^2) f_0^L(\mathbf{K}^\alpha) \tag{132}$$

or

$$f(K_{\text{nn}}, h) \geqslant -(1/2 \times 4^\alpha)\left[\ln 2 + K_0^\alpha + \sum_{i>0} |K_i^\alpha| s_i(z)\right] = f_\alpha^L(K_{\text{nn}}, h) \tag{133}$$

Equation (133) gives bounds for $\alpha = 1, 2, \ldots, NI + 1$.

Table III gives an example of such a calculation of lower bounds to the free energy. The values of the p's in the successive iterations are listed in the

Table III. Outline of a Free Energy Calculation[a]

Iteration number α	Parameter value p	Coupling constants before iteration v_2	Coupling constants before iteration v_4	Bound on free energy from Eq. (130) f_α^L
0	0.766	0.118	−0.027	−0.94487
1	0.766	0.088	p.000	−0.89581
2	0.766	0.027	0.024	−0.89035
3	0.766	−0.073	0.039	−0.89391
4	0.766	−0.139	0.062	−0.89572
5	0.766	−0.158	0.080	−0.89624
6	0.766	−0.163	0.085	−0.89638
⋮				
∞	0.766	−0.165	0.086	−0.89642

[a] The starting point is a Hamiltonian with only nearest-neighbor interactions and $K_{\text{nn}} = 0.4$. An initial decimation [see Eq. (125)] produces the couplings shown in the first row. Successive iterations using a parameter value of 0.766 give the couplings shown in the succeeding rows. The last column of the table shows the free energy bounds calculated via Eq. (130) after α steps of iteration.

Table IV. Free Energy Calculated with Adjustable Parameters[a]

Iteration number α	Parameter value p	Coupling constants before iteration v_2	v_4	Bound on free energy from Eq. (130) f_α^L
0	0.656	0.118	−0.027	−0.94487
1	0.557	0.094	−0.010	−0.89437
2	0.408	0.060	−0.002	−0.88493
3	0.221	0.022	-8.7×10^{-5}	−0.88396
4	0.067	0.002	-7.7×10^{-8}	−0.88393
5	0.033	2.07×10^{-5}	1.4×10^{-9}	−0.88393
⋮				
∞	0	0	0	−0.88343

[a] The same as Table III except that the parameters have been adjusted to give the maximum possible bound on the free energy.

table. At this moment consider them to be free parameters. The starting Hamiltonian was taken to have $K_{nn} = 0.4$ and zero magnetic field. (Note that the critical value of K_{nn} is 10% higher than this, i.e., 0.44.) After a few iterations, the K_i approach a stable fixed point, which represents the weak coupling fixed point, and then the lower bound to the exact free energy settles down to a value close to −0.89642. However, Table III does not represent the optimal calculation of the free energy. It is possible to choose p_α that

Table V. Optimal Free Energy Calculation for $K_{nn} > K_c$[a]

Iteration number α	Parameter value p	Coupling constants v_2	v_4	Bound on free energy f_α^L
0	0.871	0.165	−0.051	−1.11079
1	0.967	0.181	−0.036	−1.04819
2	1.179	0.216	−0.029	−1.03219
3	1.610	0.287	−0.014	−1.02814
4	2.252	0.401	0.107	−1.02712
5	2.465	0.561	0.451	−1.02687
6	2.466	1.034	−0.638	−1.02680
7	2.437	1.146	−0.973	−1.02679
8	2.604	1.132	−0.958	−1.02678
⋮				
∞	—	—	—	−1.02678

[a] To construct this table, one starts from a $K_{nn} = 0.5$. The free energy is then calculated with optimized parameters as shown here.

produce a greater lower bound. These optimal p's may be discovered by a numerical search procedure. The result of this optimal lower bound calculation is shown in Table IV. Notice that for large α both the couplings (K_i^{α}, for $i > 0$) and the parameters p_{α} go to zero. The net result is that after many iterations for $T < T_c$ a weak coupling ($\mathbf{K}^* = 0$) fixed point is approached. The lower bound to the free energy per site is -0.88393. The exact result is -0.87936, so that there is an error of 0.5%.

A corresponding calculation for $K_{nn} = 0.5$ with adjusted p values is shown in Table V. The lower bound to f derived from this calculation, -1.0628, agrees well with the exact result, -1.0258. In Table V, it is also interesting to notice that, for large α, p_{α} and K^{α} grow toward a strong coupling fixed point with $p \to \infty$ and $K_2 \to \infty$. The appearance of different stable

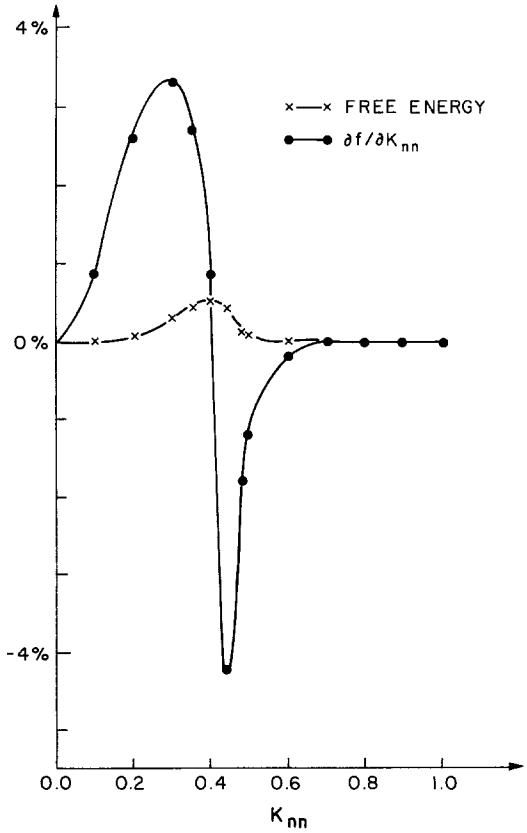

Fig. 5. Percentage errors in the calculation of free energy and $\partial f/\partial K_{nn}$. The greatest lower bound is compared with the Onsager solution. The points mark the data; the curves are only drawn as aids for the eye.

strong coupling and weak coupling fixed points accounts for the appearance of a spontaneous magnetization when K_{nn} lies above some critical value.

Calculations like those shown in Tables III–V enable us to find a function $f^L(K_{nn}, h)$ that gives the best lower bound to $f(K, h)$ that can be found within our calculational scheme. This lower-bound free energy has a singularity at $K_{nn} = 0.456$, in comparison with the exact critical value 0.4407. Figure 5 plots the ratio of the approximate free energy function to the exact one and the ratio of their derivatives with respect to K_{nn}. (The latter is twice the nearest-neighbor spin correlation function.) The maximum error in the former is 0.5%; the error in the latter has a maximum of 4.5%—which appears to be largely a result in the error in T_c. Figure 6 shows a somewhat more sensitive test of the accuracy of our approximation: a plot of $-\partial^2 F/\partial K_{nn}^2$ versus K_{nn}. This quantity differs from the specific heat by a factor of K_{nn}^2. Our results do indeed reproduce the specific heat curve reasonably well.

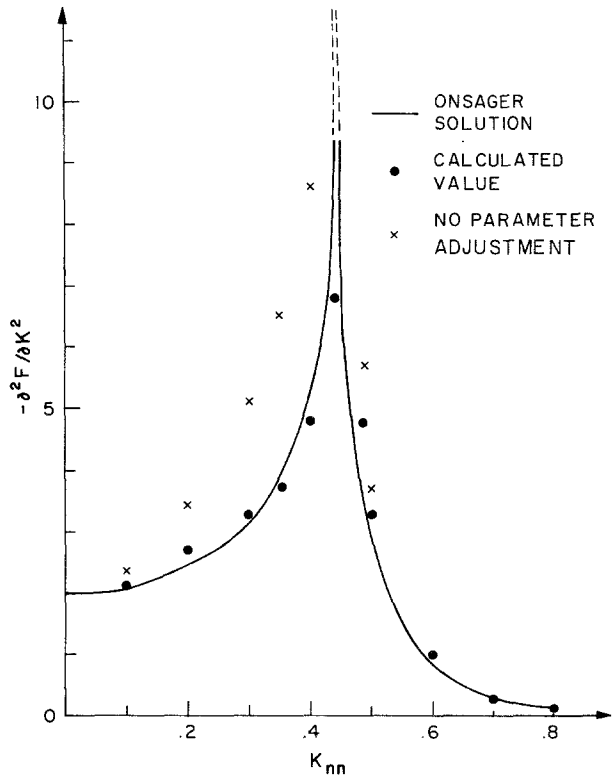

Fig. 6. Calculated $\partial^2 F/\partial K^2$ compared with the Onsager solution. The dots represent our calculation. The crosses represent a calculation in which the second derivatives are calculated at fixed values of the parameters (see Section 4.3).

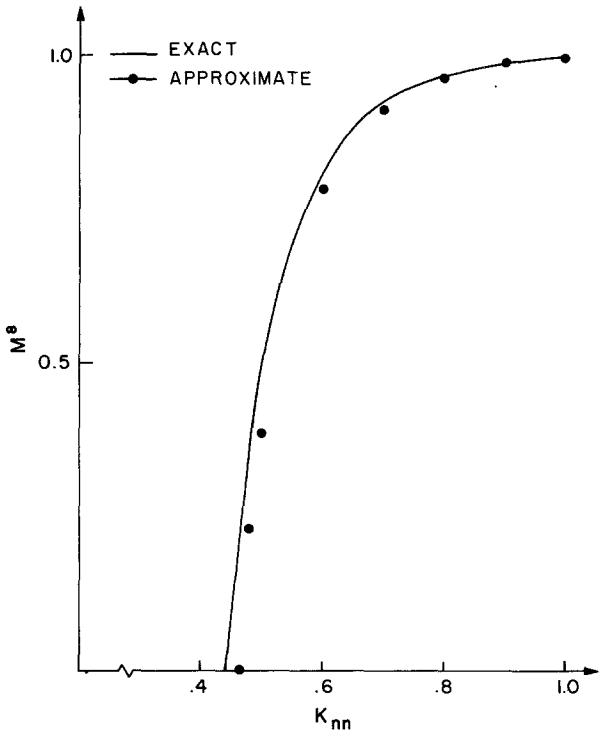

Fig. 7. Values of M^8 from the present paper compared with Yang's exact results.

Figure 7 shows a plot of the spontaneous magnetization

$$M = -\frac{\partial f(K_{nn}, h)}{\partial h}\bigg|_{h\to 0+}$$

versus K. It is presented as a plot of M^8 versus K because both the approximate and the exact solution fit $M \sim (T_c - T)^{1/8}$ very well in the critical region. Note that the error in the approximate solution can once again be ascribed mostly to an error in T_c.

Table VI shows the derived values of

$$\chi = -[\partial^2 F(K_{nn}, h)/\partial h^2]_{h=0} \tag{134}$$

listed as a function of K_{nn}. Since χ should be of the form

$$\chi = \begin{cases} C_-\left(\dfrac{K_c}{K_{nn} - K_c}\right)^{1.75} & \text{for} \quad K_{nn} > K_c \\ C_+\left(\dfrac{K_c}{K_c - K_{nn}}\right)^{1.75} & \text{for} \quad K_{nn} < K_c \end{cases} \tag{135}$$

Table VI. Values of χ and χ_{red}[a]

K_{nn}	χ	χ_{red}
0	1.0	1.0
0.1	1.57	1.017
0.2	3.00	1.089
0.3	6.87	1.064
0.35	13.60	1.078
0.4	41.94	1.118
0.44	354.69	1.193
0.48	7.08	0.0357
0.50	2.18	0.0339
0.6	0.13	0.0173
0.7	0.03	0.0106
0.8	0.01	0.0074
0.9	0.003	0.0037
1.0	0.001	0.0025

[a] Here χ_{red} is calculated from the approximate critical coupling $K_c = 0.45768$.

in the critical region, we also list the values of

$$\chi_{red} = \chi \left| \frac{K_c}{K_{nn} - K_c} \right|^{1.75} \tag{136}$$

From these values, we estimate

$$\frac{C_+}{C_-} \approx 33$$

which compares well with the series value[15]

$$\frac{C_+}{C_-} \approx 37$$

4.3. An Internal Contradiction

The reader has probably noted that our calculations have one very serious internal contradiction. In Section 4.1, where we calculated critical indices, we kept p fixed at the critical value p^*. In Section 4.2, we varied p as

the coupling constant departed from the fixed point value. As we saw in our comparison of Tables III and IV, the adjustment of p from its critical value to optimal values corresponding to the actual couplings present produces a small—but detectable—improvement in free energy values. This kind of adjustment produces relatively small changes in $\partial f/\partial K_{nn}$ near the critical point. However, $\partial^2 f/\partial K_{nn}^2$ is much more sensitive to an adjustment of the p's to the optimal values. To see this, consider Fig. 6. In this figure the x's reflect a second derivative of f with respect to K_{nn} computed at fixed p values. The values are those that are optimal for the calculation of f. The correct calculation is indicated by the dots. In this case, the p's are allowed to vary with the change in coupling. The figure shows that the correct adjustment of the p's is required to give a good fit to the specific heat.

Thus, one can see the following contradiction:

A change of the p's with a change in K's is required to give a good specific heat value, but eigenvalues calculated at fixed p are very accurate. Furthermore, we have found no natural way of computing reasonable values of $\partial p/\partial \mathbf{K}$ when $\mathbf{K}$ is very close to the critical values.

We do not understand this contradiction. For this reason, we do not understand why the eigenvalues we have calculated are so accurate. Further work will be required to understand this difficulty and to appreciate the reason for the accuracy of the eigenvalue calculations reported here.

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