PHYSICAL REVIEW B VOLUME 27, NUMBER 3 1 FEBRUARY 1983

Unified renormalization-group approach to the thermodynamic and ground-state properties of quantum lattice systems

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(Received 10 May 1982; revised manuscript received 18 October 1982)

It is shown that some recently proposed iterative approaches to the ground state of quantum systems can be obtained as zero-temperature limits of free-energy-preserving renormalization transformations, if the perturbative expansion is handled in the appropriate way. Besides giving new insight into the ground-state approaches and their mutual relationships, these results allow us to perform consistent approximate calculations of the free energy at all temperatures and to get global descriptions of the critical properties. Free-energy and specific-heat calculations are reported for XY and Heisenberg spin-$\frac{1}{2}$ chains and for the triangular XY model. It is also demonstrated how this extension into finite temperatures allows us to compute in a consistent way the z exponent, and to obtain substantial improvement in the numerical values for the ground-state energy density of the transverse Ising model.

I. INTRODUCTION

The study of quantum models is quite important for the theory of phase transitions. In these systems thermal fluctuations produce finite-temperature critical phenomena, just as in the classical systems. In addition, quantum fluctuations associated with the noncommutativity of the variables can lead to essentially new features of the thermodynamic behavior, especially at low temperatures, where thermal fluctuations become less important.

Quantum fluctuations alone can even determine zero-temperature critical phenomena in the ground state of a model.[1] The quantum critical behavior of some d-dimensional quantum models at zero temperature also turns out to be the same as that of corresponding $(d+1)$-dimensional classical systems at finite temperature; this last feature is, of course, very important for applications.

This work deals with some recently developed real-space renormalization-group methods for the study of quantum systems on lattices.[2] In the literature on the subject one can trace a clear distinction between two different main kinds of approaches. In the first category fall methods more directly inspired by analogous work performed on classical systems.[3] Such approaches[4–9] were originally proposed for the study of quantum systems at finite temperature, and they mostly made use of approximation schemes expected to be good only at high temperatures. As in the classical case,[3] the basic goal of these techniques was that of establishing a regular free-energy–preserving mapping in the space of reduced Hamiltonians of a system; this mapping was obtained by some partial resummation over the degrees of freedom of the system. In a second, and far more numerous, category fall other approaches dealing directly and exclusively with the ground-state properties of quantum systems.[10–21] For these latter methods the connection with the techniques used in the classical case is far from clear, in general, and is only based on some formal analogies.[18,19] Apparently, there is no explicit link between the approaches of the first and of the second group.

Our main purpose here is to demonstrate the existence of such a link in all the most significant cases. Indeed, we are able to show that all the above-mentioned ground-state renormalization transformations can be recovered as zero-temperature limits of properly defined free-energy–preserving mappings of the first type, computed in a suitable cumulant approximation.

As a consequence, the zero-temperature approaches allow natural finite-temperature exten-

sions. On the basis of such extensions one thus obtains a unified description of the properties of a quantum system at all temperatures, the description being based on a unique and consistent approximation scheme. Particularly appealing in this respect is the possibility of describing the low-temperature region where the crossover from classical to quantum critical behavior possibly takes place.

We show in some examples (spin-$\frac{1}{2}$ XY and Heisenberg chains and spin-$\frac{1}{2}$ triangular XY model) that our finite temperature extension of the ground-state calculations leads to a satisfactory agreement of the thermodynamic properties with known or expected results.

From a general point of view, our results also lead to a better understanding of the different zero-temperature methods and of the relationship between them. In the case of the approach of Refs. 10 and 11, such a better understanding also allows us to compute successfully an additional zero-temperature exponent (z) and to perform more consistent ground-state energy calculations. The z exponent could never be obtained before with the method of Refs. 10 and 11.

This paper is organized as follows. In Sec. II we give a first set of results concerning the finite-temperature extension of ground-state renormalization methods for systems without external fields like the spin-$\frac{1}{2}$ XY model.[16–18] In the same section we illustrate applications of these results to Heisenberg and XY models. In Sec. III we consider the so-called SLAC renormalization-group approach,[12–15,19] which can be applied to the study of zero-temperature critical phenomena in systems like the Ising or XY model with transverse fields. For the SLAC method we also find appropriate extensions to finite temperatures. We consider some general further aspects of the SLAC method and of an important generalization[20] of it in Sec. IV. Section V is devoted to the discussion and extension of the approach of Refs. 10 and 11 and to the comparison of its results with those of the SLAC method. The comparison is also based on the new calculations of the z exponent, the crossover exponent, and of the ground-state energy for the Ising model with transverse field in one and two dimensions. The last section is devoted to general comments on the results and to a discussion of possible further developments.

II. RESULTS FOR MODELS WITH DEGENERATE CELL GROUND STATES

The ground-state properties of spin-$\frac{1}{2}$ systems, such as nearest-neighbor antiferromagnetic Heisenberg chains or two-dimensional ferromagnetic XY models, received particular attention in the recent literature.[16–18,21–23] For such models, when there are no external fields acting on the spins, specific iteration techniques have been developed for the calculation of the ground-state energy density. These techniques are based on the possibility of dividing the lattice into cells with a doubly degenerate ground state (for the case of spin $\frac{1}{2}$), and they have some formal analogies with the renormalization-group approaches in real space for classical[3] or quantum-statistical systems.[4–9] Here we will show that the connection between such iterative methods and standard real-space renormalization approaches is much deeper than a purely formal analogy.

Let us consider the specific example of a spin-$\frac{1}{2}$ XY model on a triangular lattice. The Hamiltonian of such a system can be written in the general form

$$H(\{S\})=-J_1\sum_{\langle ij\rangle_{\mathrm{NN}}}(S_i^xS_j^x+S_i^yS_j^y) -J_2\sum_{\langle ij\rangle_{\mathrm{NNN}}}(S_i^xS_j^x+S_i^yS_j^y)+\cdots , \tag{2.1}$$

where S_i^x,S_i^y are Pauli matrices and $J_1,J_2,\ldots$ are nearest neighbor (NN), second nearest neighbor (NNN),... exchange interactions, respectively.

The zero-temperature approach consists in dividing the Hamiltonian H into an unperturbed part H_0, containing the interactions within cells, into which the system has been partitioned, and a perturbation V, containing interactions between different cells.[17,18] Choosing, e.g., triangular cells of three nearest-neighbor spins, the cell lattice is also triangular and rescaled by a factor $l=\sqrt{3}$ with respect to the original lattice. With such a choice of the cells and in view of the symmetries in spin space, each cell turns out to have a doubly degenerate ground state. This Kramers doublet is interpreted in this approach as the doublet of an effective cell spin.

We have chosen to label the energy eigenstates for a cell by σ_α^z and τ_α. σ_α^z represents the eigenvalue ±1 of the cell operator sign ($\sum_{i=1}^3 S_i^z$), and $\tau_\alpha=1,2,3,4$ spans the degeneracy of this operator within each of its two eigenspaces. For each eigenstate belonging to the space with σ_α^z, there is a corresponding eigenstate with the same energy and $-\sigma_\alpha^z$, which we label by the same τ_α. By convention we assign $\tau=1$ to the ground-state doublet. Indicating by $|\sigma_\alpha^z,\tau_\alpha\rangle_\alpha$ the above-mentioned cell energy eigenstates, the unperturbed ground states of the system are the $2^{N/3}$ states (N is the number of lattice sites in the system):

$$|\{\sigma_\alpha^z\},\{1\}\rangle=\prod_{\alpha=1}^{N/3}{}^{\otimes}\,|\sigma_\alpha^z,1\rangle_\alpha , \tag{2.2}$$

where the product runs over all cells. σ_α^z, which spans the degeneracy of each cell ground state, will be identified with the eigenvalue of the z component of the effective cell spin.

Let us denote by $\vec{J}$ the set of exchange interactions between the spins, and by $E_0^0(\vec{J})$ the ground-state energy corresponding to H_0. Within the framework of Rayleigh-Schrödinger perturbation theory,[24] the determination of the ground-state energy of the system amounts to the diagonalization of a $2^{N/3}\times 2^{N/3}$ matrix, whose elements, up to second order in V, e.g., take the form

$$E_0^0(\vec{J})\delta(\{\sigma_\alpha^z\},\{\sigma_\alpha'^z\})+\langle\{\sigma_\alpha^z\},\{1\}\,|\,V\,|\,\{\sigma_\alpha'^z\},\{1\}\rangle+\left\langle\{\sigma_\alpha^z\},\{1\}\left|V\frac{P}{E_0^0(\vec{J})-H_0}V\right|\{\sigma_\alpha'^z\},\{1\}\right\rangle+\cdots\,, \tag{2.3}$$

with

$$P=1-\sum_{\{\sigma_\alpha^z\}}|\{\sigma_\alpha^z\},\{1\}\rangle\langle\{\sigma_\alpha^z\},\{1\}| \tag{2.4}$$

projecting on the excited states of H_0.

Up to a constant term $W(\vec{J})$, containing $E_0^0(\vec{J})$ and higher-order contributions, it is thus natural to interpret (2.3) as matrix elements of an effective-cell Hamiltonian of the same form as the original one, but with different interactions $\vec{J}'$.[25] This interpretation is, of course, also suggested by the meaning of the eigenvalues σ_α^z.

Once this step is made, the calculation of the ground-state energy E can be performed within an iterative scheme, formally analogous to that of renormalization-group calculations of the free energy.[26] To show how the scheme works, let us first introduce dimensionless parameters $x_i=J_i/J_1$ $(i=2,3,\ldots)$. The recursions implied by the identification of (2.3) with an effective-cell spin Hamiltonian can be expressed by

$$J_i'=R_i(\vec{J}),\quad i=1,2,\ldots \tag{2.5}$$

or, more conveniently, by

$$J_1'=J_1R_1(1,x_2,x_3,\ldots)\,, \tag{2.6a}$$

$$x_i'=\frac{R_i(1,x_2,x_3,\ldots)}{R_1(1,x_2,x_3,\ldots)},\quad i=2,3,\ldots. \tag{2.6b}$$

In terms of dimensionless quantities, defined by

$$\epsilon(x_2,x_3,\ldots)=\lim_{N\to\infty}\frac{E}{NJ_1}\,, \tag{2.7a}$$

$$w(x_2,x_3,\ldots)=\lim_{N\to\infty}\frac{W}{NJ_1}\,, \tag{2.7b}$$

where E is the ground-state energy of the whole system, we finally obtain that, in the thermodynamic limit, the following basic equation must hold:

$$\epsilon(x_2,x_3,\ldots)=w(x_2,x_3,\ldots)+\frac{1}{n}R_1(1,x_2,\ldots)\times\epsilon(x_2',x_3',\ldots)\,. \tag{2.8}$$

n is the number of spins in a cell; it is equal to 3 in our example. If some suitable boundary conditions are satisfied[3,26] the difference equation (2.8) can be solved by iteration as

$$\epsilon(x_2,x_3,\ldots)=w(x_2,x_3,\ldots)+\sum_{i=1}^{\infty}n^{-i}\left[\prod_{j=0}^{i-1}R_1(1,x_2^{(j)},\ldots)\right]w(x_2^{(i)},x_3^{(i)},\ldots)\,, \tag{2.9}$$

where $x_k^{(i)}$ is the ith iteration of x_k $(=x_k^{(0)})$ according to (2.6b).

We will now show that the above algorithm for the ground-state energy can also be obtained as the zero-temperature limit of a properly defined real-space iteration scheme for the calculation of the free energy at finite temperature. In the context of the renormalization-group approach to the thermodynamics of quantum-statistical systems, one can define a free-energy–preserving mapping from the reduced Hamiltonian βH $(\beta=1/k_BT)$ to an effective cell Hamiltonian $\beta' H'$ (constant terms included), according to the following basic equation[4,5]:

$$\langle\{\sigma_\alpha^z\}\,|\,e^{-\beta'H'}\,|\,\{\sigma_\alpha'^z\}\rangle=\mathrm{Tr}_{\{\tau_\alpha\}}\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}\,|\,e^{-\beta H}\,|\,\{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle\,, \tag{2.10}$$

where the definition of $|\{\sigma_\alpha^z\},\{\tau_\alpha\}\rangle$ is an obvious generalization of (2.2), and, as in the previous case, σ_α^z and $\sigma_\alpha'^z$ are interpreted on the left-hand side (lhs) as z components of cell spin variables.[4,5] Indeed, Eq. (2.10) implicitly defines a mapping in the space of reduced interactions $K_i=\beta J_i$ $(i=1,2,\ldots)$. In order to recover the previous zero-temperature scheme in the limit of $\beta\to\infty$, the basic step consists now in expanding the exponential on the right-hand side (rhs) of Eq. (2.10) in powers of V. To this purpose, we use the Feynman identity

$$e^{-\beta(H_0+V)}=e^{-\beta H_0}T_\mu\left[\exp\left[-\int_0^\beta d\mu\, e^{\mu H_0}Ve^{-\mu H_0}\right]\right], \tag{2.11}$$

where T_μ is the "time ordering" operator with respect to decreasing values of μ.

Expanding up to second order in V both sides of Eq. (2.10), we obtain

$$\begin{aligned}
&e^{-\beta' E_0'^0}\Big[\delta(\{\sigma_\alpha^z\},\{\sigma_\alpha'^z\})-\langle\{\sigma_\alpha^z\}\,|\,\beta' H_1'\,|\,\{\sigma_\alpha'^z\}\rangle-\langle\{\sigma_\alpha^z\}\,|\,\beta' H_2'\,|\,\{\sigma_\alpha'^z\}\rangle \\
&\quad+\tfrac{1}{2}\sum_{\{\sigma_\alpha''^z\}}\langle\{\sigma_\alpha^z\}\,|\,\beta' H_1'\,|\,\{\sigma_\alpha''^z\}\rangle\langle\{\sigma_\alpha''^z\}\,|\,\beta' H_1'\,|\,\{\sigma_\alpha'^z\}\rangle+\cdots\Big] \\
&=\mathrm{Tr}_{\{\tau_\alpha\}}e^{-\beta E_0(\{\tau_\alpha\})}\Big[\delta(\{\sigma_\alpha^z\},\{\sigma_\alpha'^z\})-\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}\,|\,\beta V\,|\,\{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle \\
&\qquad+\sum_{\{\sigma_\alpha''\},\{\tau_\alpha''\}}\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}\,|\,\beta V\,|\,\{\sigma_\alpha''^z\},\{\tau_\alpha''\}\rangle\langle\{\sigma_\alpha''^z\},\{\tau_\alpha''\}\,|\,\beta V\,|\,\{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle \\
&\qquad\times\Omega(\beta[E_0(\{\tau_\alpha''\})-E_0(\{\tau_\alpha\})])+\cdots\Big],
\end{aligned} \tag{2.12}$$

where we used the function $\Omega(x)$, defined by

$$\Omega(x)=\frac{1}{x}+\frac{e^{-x}-1}{x^2}, \qquad \Omega(0)\equiv\lim_{x\to 0}\Omega(x)=\tfrac{1}{2}. \tag{2.13}$$

In (2.12) $E_0(\{\tau_\alpha\})$ indicates the unperturbed energy levels of H_0, and $E_0(\{1\})=E_0^0(\vec{J})$ is the ground-state energy of H_0. The transformed Hamiltonian H' was also split into a zeroth-order constant term $E_0'^0$, given by

$$-\beta' E_0'^0=\ln\mathrm{Tr}_{\{\tau_\alpha\}}\exp[-\beta E_0(\{\tau_\alpha\})], \tag{2.14}$$

and in first- and second-order terms H_1' and H_2', respectively. The energy eigenvalues of H_0 depend, of course, only on the $\{\tau_\alpha\}$ configuration, as a consequence of our labeling of the states $|\sigma_\alpha,\tau_\alpha\rangle_\alpha$.

Equation (2.12) allows us to determine H' and thus its reduced couplings $\vec{K}'$ up to second order in V for all β. Furthermore, taking $\{\sigma_\alpha'^z\}=\{\sigma_\alpha^z\}$ and performing the trace with respect to $\{\sigma_\alpha^z\}$, we must obtain, after taking the logarithms and dividing by N, for N going to infinity,

$$f(\vec{K})=g(\vec{K})+\frac{1}{n}f(\vec{K}'(\vec{K})), \tag{2.15}$$

where f is the dimensionless free energy per spin in the thermodynamic limit, and g comes from an extensive constant term in H'.

The crucial point consists now in showing that Eqs. (2.10), (2.12), and (2.15) for $\beta\to\infty$ lead to the equations of the $T=0$ approach described above. Letting β go to infinity in (2.12) (this means that all K_i's on the rhs go to infinity with the same rate), the dominant contributions on the rhs are those proportional to $\exp[-\beta E_0(\{1\})]$. The argument x of the Ω function goes to infinity too, except for the degenerate cases where $E_0(\{\tau_\alpha''\})=E_0(\{\tau_\alpha\})$; in these cases $x=0$ and Ω takes on the special value $\frac{1}{2}$. Taking thus into account on both sides only the dominant contributions for $\beta,\beta'\to\infty$, we obtain asymptotically, order by order in V,

$$\beta' E_0'^0\simeq\beta E_0(\{1\}), \tag{2.16a}$$

$$\langle\{\sigma_\alpha^z\}\,|\,\beta' H_1'\,|\,\{\sigma_\alpha'^z\}\rangle\simeq\langle\{\sigma_\alpha^z\},\{1\}\,|\,\beta V\,|\,\{\sigma_\alpha'^z\},\{1\}\rangle, \tag{2.16b}$$

$$\langle\{\sigma_\alpha^z\}\,|\,\beta' H_2'\,|\,\{\sigma_\alpha'^z\}\rangle\simeq\left\langle\{\sigma_\alpha^z\},\{1\}\left|\beta V\frac{P}{\beta E_0(\{1\})-\beta H_0}\beta V\right|\{\sigma_\alpha'^z\},\{1\}\right\rangle, \tag{2.16c}$$

where (2.16a), (2.16b), and (2.16c) refer to zeroth, first, and second order, respectively.

It is immediately clear that Eqs. (2.16) imply asymptotically for the K_i's the transformation

$$K_i'\simeq R_i(\vec{K}),\quad i=1,2,3,\ldots \tag{2.17}$$

where the R_j functions are the same as those in (2.5). Equations (2.16) also imply that, for β going

to infinity,

$$g(\vec{K}) \simeq K_1 w(x_2, x_3, \ldots) , \tag{2.18}$$

where w is the same function appearing in Eq. (2.8). Dividing then Eq. (2.15) by K_1 and taking the limit of $\vec{K}$ going to infinity ($x_i = K_i/K_1$ fixed), we obtain a recursion formula for the dimensionless ground-state energy $\epsilon(x_2, x_3, \ldots)$. Taking into account (2.5), (2.6), and (2.16)–(2.18), we finally realize that (2.15) is converted in this way exactly into the form (2.8) with $x_2', x_3', \ldots$ given by (2.6b). For this result we use the fact that the limit of f/K_1, for β going to infinity, must be equal to ϵ. This shows that the renormalization approach just described reduces to the iterative scheme of Refs. 17 and 18 in the limit of zero temperature.

A natural question concerning the above result is whether the technique for the finite-temperature renormalization mapping is unique or not. The answer is that there are certainly many different renormalization transformations with the same limit property of reducing to the given ground-state approach. One could indeed make a somewhat different choice of the states $|\sigma_\alpha, \tau_\alpha\rangle$ in each cell. If these states are chosen not to coincide with energy eigenstates, but with orthonormal combinations of them, one can obtain a different finite-temperature transformation, having however the same limit for T approaching zero. The only requirement on the linear combinations is that they do not mix $\sigma_\alpha^z = +1$ with $\sigma_\alpha^z = -1$ eigenspaces, and that for a given τ the $\sigma_\alpha^z = +1$ state is obtained from the $\sigma_\alpha^z = -1$ state by reversing all the z components of the spins in the cell.

We now want to show some examples of how this finite-temperature extension of the ground-state method allows us to make consistent approximate calculations of the free energy at all temperatures. Of course, as we will see, this can be more or less difficult, according to the degree of complication of the thermodynamic behavior of the system at finite temperatures (e.g., presence or absence of critical singularities). We performed free energy and specific heat calculations on one-dimensional models for which exact (spin-$\frac{1}{2}$ XY chain) or numerical (spin-$\frac{1}{2}$ Heisenberg chain) results are available for comparison. For such systems the extension of the ground-state iterative calculations is rather straightforward and very successful, already in first-order schemes.

The agreement of our first-order free-energy calculations on quantum chain systems with exact[27] or independent numerical[28] results is quite satisfactory for all temperatures. Indeed, on a percentile basis, our free energies deviate not more from the expected values than the corresponding iterative ground-state energies. In the case of the ferromagnetic XY chain, e.g., with a three-spin cell transformation, the maximum percentual deviation of our free energy from the exact one is about 13%, whereas the ground-state energy deviates by 11%.[2] As an illustration of our results, we compare in Fig. 1 the specific heat of the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain, obtained by our method (three-spin cell first-order transformation), with the values extrapolated numerically by Bonner and Fischer[28] on the basis of finite-chain calculations (up to 11 spins). As one can see, the behavior of our results for specific heat is particularly satisfactory, especially at low temperatures.

These results show that our finite-temperature extensions are very meaningful and successful for one-dimensional systems, which are the object of most applications of ground-state renormalization. Here we also want to discuss the relatively more complicated situation arising when we try to get a global thermodynamic description of a highly nontrivial model like the two-dimensional ferromagnetic XY model, for which series expansions[29,30] and renormalization approaches[4–6,9] give evidence for the existence of a critical transition at finite temperature. The presence of a singular behavior in the free energy at a finite temperature makes it more difficult to find approximations that are acceptable both at high and low temperatures.

A first attempt to an iterative computation of the ground-state energy of the triangular spin-$\frac{1}{2}$ XY model was done by one of the present authors[17] on the basis of the $T=0$ method of Ref. 16. In Ref. 17

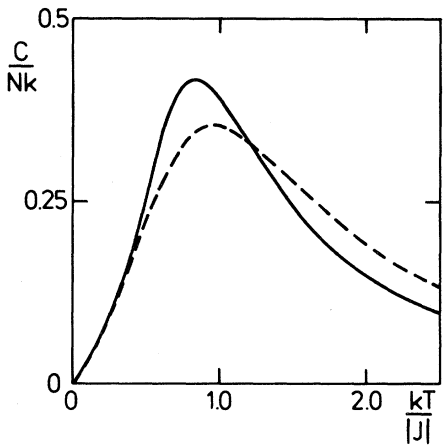

FIG. 1. Specific heat for the antiferromagnetic Heisenberg chain vs temperature; the solid curve represents the results from our iterative calculation, the dotted curve shows the numerical extrapolation from Ref. 28.

the system was divided in three-spin triangular cells, as described in the beginning of this section, and the perturbational part of H, V, was initially taken to be equal to the sum of all interactions among spins of different cells. In contrast to what happens in analogous calculations with one-dimensional models, the standard ground-state calculation scheme was, however, giving a rather strong deviation of the second-order result, as compared to the first-order result.[31] Furthermore, this second-order result turned out to disagree, quite sensibly, with the independent estimates of Refs. 22 and 23.

This suggested[17] the modification of the perturbation scheme by introducing a different separation of H into unperturbed and perturbed parts. Indicating by H_0 and V the previous terms, one might replace them by

$$\tilde{H}_0=\lambda H_0 , \tag{2.19}$$

$$\tilde{V}=V+(1-\lambda)H_0 , \tag{2.20}$$

with λ being a parameter to be determined. The separation (2.19) and (2.20), which reduces to the standard one for $\lambda=1$, was made in the hope of "reducing" the relative strength of the perturbation V. A very simple qualitative argument of topological nature would suggest a value of λ around 3 for specifying a "good" splitting of H.[17]

The second-order results based on (2.19) and (2.20) are rather sensitive to the choice of λ. It turns out that one has to choose $\lambda\simeq 2.3$ in order to be in strict agreement with the results of Refs. 22 and 23.

The free energy of the XY model with nearest-neighbor interaction J_1 on the triangular lattice is rather well known at high temperatures through its series expansion in $K_1=\beta J_1$.[32] By iteration of (2.15), we can show that our method in a second-order cumulant expansion agrees exactly with the series expansion of the free energy up to second order in K_1, independently from the choice of λ. Higher-order terms in K_1, however, are reproduced only approximately, and for every value for K_1 we can determine an optimal value $\lambda(K_1)$ such that our iteration procedure reproduces exactly the free-energy value obtained by applying the standard Padé analysis on the series expansion. In Fig. 2 we have plotted this optimal $\lambda(K_1)$ within the confidence region of the Padé analysis, as a function of $\exp(-2K_1)$, which is the natural expansion parameter for our iteration scheme. We see that this optimal value tends to $\lambda\simeq 1.5$ for high temperatures, while somewhat smaller values have to be used for lower temperatures. At lower temperatures, however, the Padé results start becoming doubtful, due to the approach of the critical point.

Very little is known about the low-temperature thermodynamic properties of the two-dimensional XY model, except for some numerical estimates of the ground-state energy ϵ. In applying our iteration scheme (2.8), our predictions for ϵ are again λ dependent, as shown in Fig. 3. As we said already, in order to agree with the estimate $\epsilon\simeq -1.58$ for the triangular lattice,[22,23] we should use $\lambda\simeq 2.3$. The deviation from this expected result is rather limited as long as $\lambda\gtrsim 1.5$, but it becomes much stronger for λ values around 1.0.

Since both the high- and low-temperature thermodynamic behavior are qualitatively well described by

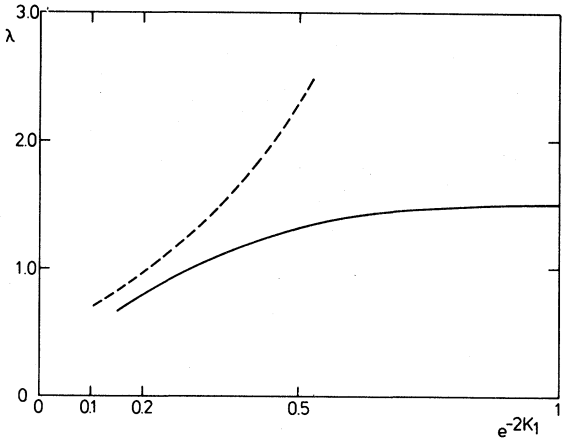

FIG. 2. Solid curve shows the optimal values $\lambda(K_1)$ for choosing the perturbational part of the Hamiltonian, according to (2.20), as a function of $\exp(-2K)=\exp(-2\beta J_1)$. Optimalization is obtained by comparing the free energy from iterating (2.15) with results from series expansions, for the XY model on the triangular lattice. Dotted line shows the critical points $K_c(\lambda)$.

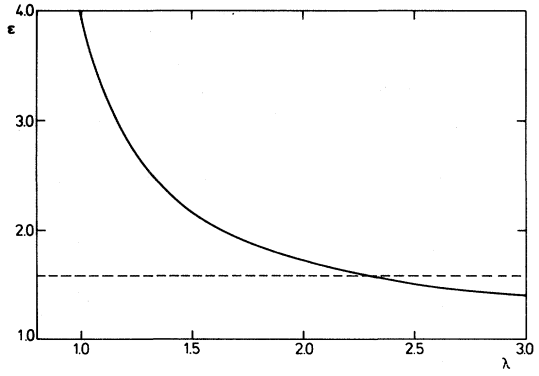

FIG. 3. Ground-state energy ϵ per lattice site, as defined in (2.7), obtained from our iteration scheme (2.8), as a function of the parameter λ. Dotted level represents the numerical estimate obtained for ϵ in Refs. 22 and 23, and this is reproduced in our scheme with $\lambda\simeq 2.3$.

a choice of λ in the range $1.5 \leq \lambda \leq 2.5$, it is very tempting to assume that a fixed choice for λ in this interval may give, at least qualitatively, a correct description of the whole temperature range. For every λ we have a critical point $K_c(\lambda)$ such that for all $K_1 < K_c$ the repeated iteration (2.17) on $\vec{K}=(K_1,0,0,\ldots)$ leads ultimately to the infinite temperature fixed point $\vec{K}^*=(0,0,0,\ldots)$, whereas it tends to infinity (the zero-temperature fixed point) for $K_1 > K_c$. This relation between λ and the critical value K_c has also been displayed in Fig. 2.

For the specific choice $\lambda=1.5$, we have $K_c(1.5)\simeq 0.52$, and K_c decreases slightly with increasing λ. According to high-temperature series analysis, the transition could tentatively be located[29] at $K_c \simeq 0.76$ when one assumes a power-law singularity in the magnetic susceptibility, but this estimate is not very reliable and could radically change if an exponential singularity were assumed.[30]

It is interesting to note that within our approximation the specific heat turns out to diverge for $K \to K_c$, with an exponent $\alpha \simeq 0.25$, a result which is rather insensitive to variations of λ in the interval $1.5 \leq \lambda \leq 2.5$. It is important to stress here that our approximation is able to give a qualitatively satisfactory description of the system at all temperatures, even if the location and the nature of critical singularities are probably reproduced rather roughly.

III. FINITE-TEMPERATURE EXTENSION OF THE SLAC APPROACH

In this section we will focus our attention on a particular zero-temperature renormalization method, which can be used in the interesting case of nondegenerate cell ground states. This technique, originally inspired by the Wilson approach to the Kondo effect,[33] can be seen as an iterative approximate method for the construction of the ground state of a system. In the form presented here, the method was first proposed by Jafarey *et al.*,[34] and later strongly developed by Drell *et al.* for problems of lattice theory.[12] A detailed discussion of this so-called SLAC method is beyond the purpose of this paper. Here we will recall very briefly the basic definitions, using the spin-$\frac{1}{2}$ Ising model with transverse field as an example.

This model is described by a Hamiltonian of the form

$$H = -J \sum_{\langle ij \rangle} S_i^x S_j^x - \Gamma \sum_i S_i^z , \tag{3.1}$$

where J is an exchange Ising-type interaction and Γ is the transverse field. S_i^x and S_j^z are Pauli spin operators. In (3.1) the sum over i and j is restricted for the moment to couples of nearest-neighbor sites.

The construction of the renormalized Hamiltonian with the SLAC method is again based on a division of the system into cells and on a separation of H into an intracell and an intercell part.[19] Our discussion, at least for the moment, is general and does not depend on the space dimensionality or on the cell division. Owing to the presence of the field Γ, the ground state of the single-cell Hamiltonian is nondegenerate. The idea of the SLAC method is that of identifying the ground state and the first excited state of a cell with the eigenstates of the cell spin component σ_α^z, respectively, parallel and antiparallel to the direction of the transverse field. Let us indicate such states of a cell by $|\sigma_\alpha^z,1\rangle_\alpha$, with $\sigma_\alpha^z = \pm 1$ for the ground state and first excited state, respectively ($\Gamma > 0$).

The mapping from H to H' is then obtained by projecting H on the subspace of the Hilbert space spanned by all the states of the form

$$|\{\sigma_\alpha^z\},\{1\}\rangle = \prod_\alpha{}^{\otimes} |\sigma_\alpha^z,1\rangle_\alpha , \tag{3.2}$$

and by making the formal identification

$$\langle \{\sigma_\alpha^z\} | H' | \{\sigma'^z_\alpha\} \rangle = \langle \{\sigma_\alpha^z\},\{1\} | H | \{\sigma_\alpha'^z\},\{1\} \rangle , \tag{3.3}$$

where on the lhs the σ_α^z's are interpreted as cell spin component eigenvalues. Clearly in (3.3) H_0, the intracell part of the interaction, defines the new magnetic field Γ', according to

$$-\left[E_0'^0(J,\Gamma)+\Gamma' \sum_\alpha \sigma_\alpha^z\right] = \langle \{\sigma_\alpha^z\},\{1\} | H_0 | \{\sigma_\alpha^z\},\{1\} \rangle , \tag{3.4}$$

whereas the intercell part, which is off-diagonal in the basis (3.2), defines J' according to

$$\left\langle \{\sigma_\alpha^z\} \left| -J' \sum_{\langle \alpha\beta \rangle} \sigma_\alpha^x \sigma_\beta^x \right| \{\sigma'^z_\alpha\} \right\rangle = \langle \{\sigma_\alpha^z\},\{1\} | V | \{\sigma_\alpha'^z\},\{1\} \rangle . \tag{3.5}$$

$E_0'^0$ plays the same role as the quantity W that we met in the preceding section, whose presence allows an iterative calculation of the ground-state energy.

For obtaining the ground-state mapping based on Eqs. (3.4) and (3.5) as the $\beta \to \infty$ limit of a finite-temperature renormalization transformation, we proceed as follows. If the number of spins in our αth cell is $n = l^d$, let us label the remaining $2^n - 2$ energy eigenstates, besides $|1,1\rangle_\alpha$ and $|-1,1\rangle_\alpha$, by

assigning to half of them $\sigma_\alpha^z=+1$ and $\tau_\alpha=2,3,4,\ldots,2^{n-1}$ and to the other half $\sigma_\alpha^z=-1$ and the same range of τ values. For the moment we do not discuss the specific labeling conventions; we will come back to this at the end of this section. Having defined our $|\sigma_\alpha,\tau_\alpha\rangle_\alpha$ states for the cells, we define a finite-temperature renormalization mapping for the system, in analogy with what we did in the preceding section, according to

$$\langle\{\sigma_\alpha^z\}|e^{-\beta' H'}|\{\sigma_\alpha'^z\}\rangle = \mathrm{Tr}_{\{\tau_\alpha\}}\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}|e^{-\beta H}|\{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle\ . \tag{3.6}$$

Let us first expand $e^{-\beta H}$ on the rhs of (3.6) up to first order in V (V being the intercell interaction) on the basis of (2.11). In this way we obtain

$$\mathrm{Tr}_{\{\tau_\alpha\}}\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}|e^{-\beta(H_0+V)}|\{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle$$
$$=\mathrm{Tr}_{\{\tau_\alpha\}}e^{-\beta E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})}[\delta(\{\sigma_\alpha^z\},\{\sigma_\alpha'^z\})-\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}|\beta V|\{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle$$
$$\times\chi(\beta E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})-\beta E_0(\{\sigma_\alpha'^z\},\{\tau_\alpha\}))]\ , \tag{3.7}$$

where

$$\chi(x)=\frac{1}{x}(e^x-1),\quad \chi(0)=\lim_{x\to 0}\chi(x)=1\ . \tag{3.8}$$

In (3.7) $E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})$ represents the eigenvalue of the intracell Hamiltonian H_0, which now depends also on $\{\sigma_\alpha^z\}$.

If we make an analogous expansion on the lhs of (3.6), splitting $\beta' H'$ into a zeroth-order part $\beta' H_0'$ diagonal in the $|\{\sigma_\alpha^z\}\rangle$ basis, and in a first-order part $\beta' H_1'$, we obtain

$$\langle\{\sigma_\alpha^z\}|e^{-\beta' H'}|\{\sigma_\alpha'^z\}\rangle=e^{-\beta' E_0'(\{\sigma_\alpha^z\})}[\delta(\{\sigma_\alpha^z\},\{\sigma_\alpha'^z\})-\langle\{\sigma_\alpha^z\}|\beta' H_1'|\{\sigma_\alpha'^z\}\rangle$$
$$\times\chi(\beta' E_0'(\{\sigma_\alpha^z\})-\beta' E_0'(\{\sigma_\alpha'^z\}))]\ , \tag{3.9}$$

where $\beta' E_0'(\{\sigma_\alpha^z\})$ are the eignevalues of $\beta' H_0'$, which must have the form

$$\beta' E_0'(\{\sigma_\alpha^z\})=\beta' E_0'^0+\beta'\Gamma'\sum_\alpha\sigma_\alpha^z\ , \tag{3.10}$$

if we compare the zeroth-order terms of (3.7) and (3.9). Of course $E_0'^0$ and Γ' in (3.10) do not satisfy (3.4), but a finite-temperature generalization of this formula, analogous to (2.14). Equations (3.7), (3.9), and (3.10) fully determine $\beta' H'$ up to first order in V, for all temperatures. We now consider the $\beta\to\infty$ limit for this finite-temperature mapping.

Since in our construction $E_0(\{\sigma_\alpha^z\},\{1\})$ is always the lowest energy compatible with a given $\{\sigma_\alpha^z\}$ configuration, in (3.7) only the term with $\{\tau_\alpha\}=\{1\}$ will dominate in the trace over $\{\tau_\alpha\}$, when $\beta\to\infty$. So asymptotically for very large β we obtain

$$\beta' E_0'(\{\sigma_\alpha^z\})\simeq\beta E_0(\{\sigma_\alpha^z\},\{1\})\ , \tag{3.11}$$

for the zeroth-order terms, and

$$\langle\{\sigma_\alpha^z\}|\beta' H_1'|\{\sigma_\alpha'^z\}\rangle \simeq\langle\{\sigma_\alpha^z\},\{1\}|\beta V|\{\sigma_\alpha'^z\},\{1\}\rangle \tag{3.12}$$

for the first-order terms.

Equations (3.10)–(3.12) show that, if we indicate by

$$J'=R_1(J,\Gamma)\ , \tag{3.13a}$$

$$\Gamma'=R_2(J,\Gamma) \tag{3.13b}$$

the zero-temperature transformation of the SLAC approach, as determined by (3.4) and (3.5), our finite-temperature renormalization mapping becomes, for $\beta\to\infty$,

$$K_1'\simeq R_1(K_1,K_2)\ , \tag{3.14a}$$

$$K_2'\simeq R_2(K_1,K_2)\ , \tag{3.14b}$$

with $K_1=\beta J$, $K_2=\beta\Gamma$. In addition, one finds

$$\beta' E_0'^0\simeq\tfrac{1}{2}[\beta E_0(\{+1\},\{1\}) +\beta E_0(\{-1\},\{1\})]\ . \tag{3.14c}$$

As in the previous case of the XY model, we thus discover that the first-order free-energy transformation equation consistent with (3.6) reduces exactly to the SLAC equation for the ground-state energy per spin in the $\beta\to\infty$ limit.

A mapping like (3.14) is expected to have a zero-temperature fixed point for a given value x^* of the

ratio $x=\Gamma/J=K_2/K_1$ when the dimensionless temperature $T=K_1^{-1}$ becomes zero. Asymptotically, for T approaching zero, we can write for these dimensionless parameters on the basis of (3.14)

$$x' \simeq f(x)=\frac{R_2(1,x)}{R_1(1,x)} , \tag{3.15a}$$

$$\frac{T'}{T} \simeq R_1^{-1}(1,x) . \tag{3.15b}$$

This shows that, for $x=x^*$ [$f(x^*)=x^*$], we have

$$\lim_{T\to 0}\frac{T'}{T} \simeq R_1^{-1}(1,x^*) . \tag{3.16}$$

$R_1^{-1}(1,x^*)$ is connected to the z exponent[1] by

$$R_1(1,x^*)=n^{-z/d}=l^{-z} . \tag{3.17}$$

The z exponent obtained in this way is indeed identical to the one computed in the SLAC approach on the basis of (3.13a) and (3.13b), if one takes into account that, for $x=x^*$, the dimensional quantities J and Γ are multiplied by a common factor at each iteration of (3.13).[19]

We have just shown that a scheme like that defined by (3.6) is indeed a consistent finite-temperature extension of the SLAC method in its standard form. *A priori* there seems to be a great deal of arbitrariness in the choice of the labeling (σ,τ) for the higher excited states of the system. These states indeed do not enter, to first order, into the zero-temperature formulas. Of course, this choice is of importance as soon as one is at finite temperatures. Some special choices may be more powerful than others in yielding a realistic picture of the overall properties of the system in a given approximation. Our conviction is that in each specific problem general symmetry considerations should lead to a natural choice of the labeling of the states.

As an example, we can briefly discuss the case of the triangular Ising model with transverse field, which has not only a zero-temperature critical point, but a whole line of critical points connecting the $T=0$ point with the classical Ising critical point ($K_1=0.2744, x=0$). In order to have a physically acceptable picture of the thermodynamic properties of the system, the classical Ising systems ($x=0$) must of course be an invariant set of the transformation. In other words, if $K_2=0$, the symmetry of the reduced Hamiltonian with respect to inversion of the z axis in spin space must be preserved. This will be guaranteed by an appropriate (σ,τ) labeling, consistent with such a symmetry. Let us, e.g., consider the case of three-spin cells in a triangular lattice. The lowest two energy eigenstates for a cell must, of course, be labeled $|+,1\rangle$ and $|-,1\rangle$ if one wants to obtain the SLAC transformation in the limit of zero temperature. For the higher-energy states one can proceed as follows. One considers an energy eigenstate and assigns to it a given σ value, consistent in sign with the average of $\sum_{i\in\alpha}S_i^z$ in that state, and e.g., $\tau=2$. The state $|-\sigma,2\rangle$ will be chosen as the state which, in the $x=0$ limit, can be obtained from $|\sigma,2\rangle$ by an inversion of the z axis. The same procedure is followed for the remaining states, until all of them have been labeled.

It is interesting to note that, proceeding in this way and choosing appropriate phase factors for multiplying the eigenstates, one can arrive at a definition of the transformation which, for the case $x=0$, exactly reduces to the first-order cumulant approximation of the Niemeijer and van Leeuwen majority rule transformation of the Ising model.[3] The specific choice that we propose according to these rules for the three-spin cell are reported in Appendix A. The renormalization flow in a (T,x) diagram is then characterized by a fixed point at $(0,x^*)$ and another one at $(T_c,0)$, where T_c is the Niemeijer–van Leeuwen fixed point.[3] $K_{1c}=T_c^{-1}=0.336$ with

$$\lambda_T=\left.\frac{dK_1'}{dK_1}\right|_{x=0,K_1=K_{1c}}=1.63 .$$

There is a critical line joining these two points, and all points on this line are attracted by the classical Ising fixed point (see Fig. 4). The zero-temperature fixed point at $(0,x^*)$ is unstable both in the x and T directions; the relevant exponents, respectively, are

$$\nu^{-1}=\frac{1}{\ln l}\ln\left[\left.\frac{\partial x'}{\partial x}\right|_{x=x^*,T=0}\right]=0.63$$

and

$$z=\frac{1}{\ln l}\ln\left[\lim_{T\to 0}\frac{T'}{T}\right]$$

$$=\frac{1}{\ln l}\ln[R_1^{-1}(1,x^*)]=0.13$$

($l=\sqrt{3}$). These exponents are, of course, the same as those given by the SLAC method.

A similar calculation performed on the $d=1$ Ising system in a transverse field shows only the presence of a zero-temperature fixed point. There is neither a critical line nor a finite-temperature fixed point on the pure Ising axis, in accordance with the expected fact that a quantum one-dimensional system should display a critical behavior only at $T=0$.[1]

Other choices of the phase factors for the energy eigenstates, different from those mentioned in Appendix A, can be seen to lead to different and poorer results for K_{1c} and λ_T. We can thus regard the

above type of choice as an optimal one for the global description of the system. In the next section we will discuss further aspects of the SLAC method, especially in connection with its perturbative generalization of Ref. 20.

IV. PERTURBATIVE GENERALIZATION OF THE SLAC APPROACH AND ITS FINITE-TEMPERATURE EXTENSION

The zero-temperature SLAC approach discussed in the preceding section also has a systematic perturbative extension in powers of the intercell interactions. Such an extension was recently obtained with a zero-temperature technique, inspired by analogous methods for the renormalization group in critical dynamics.[20]

A detailed discussion of the results of Ref. 20 is beyond the purpose of the present work. We only recall that in this paper the mapping in Hamiltonian space is constructed on the basis of the "dynamical" requirement of preserving the low-lying excited state energies of the system besides the ground-state energy. This requirement still allows a large freedom in the specification of the mapping. In Ref. 20 the zero-temperature mapping was completely determined by further imposing an *a priori* unnecessary Hermiticity condition.

In that way, the second-order correction $\langle\{\sigma_\alpha^z\}|H_2'|\{\sigma_\alpha'^z\}\rangle$ to the SLAC matrix elements of H' takes in our notations the relatively simple form

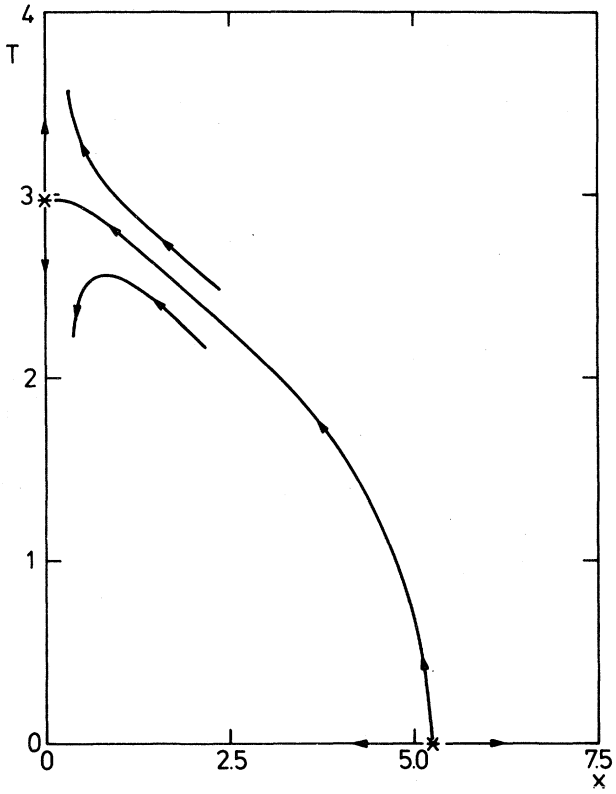

FIG. 4. Renormalization flow obtained for the two-dimensional transverse Ising model. On the axes are $x=\Gamma/J$ and $T=K^{-1}$. The unstable fixed point is at $(x^*=5.25, T=0)$ and the Ising fixed point at $(x=0, T^*=2.98.)$.

$$\langle\{\sigma_\alpha^z\}|H_2'|\{\sigma_\alpha'^z\}\rangle=\frac{1}{2}\sum_{\substack{\{\sigma_\alpha''^z\},\{\tau_\alpha''\}\\(\{\tau_\alpha''\}\neq\{1\})}}\langle\{\sigma_\alpha^z\},\{1\}|V|\{\sigma_\alpha''^z\},\{\tau_\alpha''\}\rangle\langle\{\sigma_\alpha''^z\},\{\tau_\alpha''\}|V|\{\sigma_\alpha'^z\},\{1\}\rangle$$
$$\times\left[\frac{1}{E_0(\{\sigma_\alpha^z\},\{1\})-E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\})}+\frac{1}{E_0(\{\sigma_\alpha'^z\},\{1\})-E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\})}\right],\tag{4.1}$$

which, e.g., applies to the Ising model with transverse field of the preceding section.

In view of the results obtained until now, our zero-temperature–limit procedure applied to free-energy–preserving mappings should provide a very natural way of defining and computing perturbative generalizations of the SLAC method. In other words, we hope to convert our finite-temperature perturbative expansion into a zero-temperature one, by taking the limit $\beta\to\infty$ in an appropriate way, just as we did for the pure XY model. This turns out to be possible, ultimately, but the situation is more complicated now, in comparison with the case of Sec. II.

The simple definition (3.6) of the finite-temperature transformation in terms of unperturbed energy eigenstates does not allow us to obtain consistently an expansion in powers of V for the limit

mapping. The results obtained by using the $\beta \to \infty$ limit on a second-order approximation of (3.6) are not compatible with the SLAC transformation, which was obtained in first order.

Let us analyze in more detail the situation in second order. For computing the asymptotic behavior of the matrix elements

$$\langle \{\sigma_\alpha^z\} \mid \exp(-\beta' H') \mid \{\sigma_\alpha'^z\} \rangle$$

in (3.6), we must first determine which exponential function of unperturbed energies dominates in the limit $\beta \to \infty$ for the given $\{\sigma_\alpha^z\}$ and $\{\sigma_\alpha'^z\}$. A nice feature of the first-order case was that, for every choice of $\{\sigma_\alpha^z\}$ and $\{\sigma_\alpha'^z\}$, the dominant exponential was either

$$\exp[-\beta E_0(\{\sigma_\alpha^z\},\{1\})]$$

or

$$\exp[-\beta E_0(\{\sigma_\alpha'^z\},\{1\})] ,$$

according to whether $E_0(\{\sigma_\alpha^z\},\{1\})$ or $E_0(\{\sigma_\alpha'^z\},\{1\})$ was the lower energy. In second order this property drastically disappears and, regardless of $\{\sigma_\alpha^z\}$ and $\{\sigma_\alpha'^z\}$, the dominant exponential is that of the unperturbed ground-state energy $E_0(\{\bar{\sigma}\},\{1\})$ whenever this ground state appears as an intermediate state in the second-order perturbative term ($\{\bar{\sigma}\} = \{+1\}$ with $\Gamma > 0$).

In Appendix B we report the full expressions for a second-order approximation to Eq. (3.6). On the basis of these expressions. one gets the following equations for the matrix elements of H' ($= H_0' + H_1' + \cdots$) in the limit $\beta \to \infty$:

$$\frac{\langle \{\sigma_\alpha^z\} \mid H_1' \mid \{\bar{\sigma}\} \rangle \langle \{\bar{\sigma}\} \mid H_1' \mid \{\sigma_\alpha'^z\} \rangle}{[E_0'(\{\bar{\sigma}\}) - E_0'(\{\sigma_\alpha^z\})][E_0'(\{\bar{\sigma}\}) - E_0'(\{\sigma_\alpha'^z\})]}$$

$$= \sum_{\{\tau_\alpha\}} \frac{\langle \{\sigma_\alpha^z\},\{\tau_\alpha\} \mid V \mid \{\bar{\sigma}\},\{1\} \rangle \langle \{\bar{\sigma}\},\{1\} \mid V \mid \{\sigma_\alpha'^z\},\{\tau_\alpha\} \rangle}{[E_0(\{\bar{\sigma}\},\{1\}) - E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})][E_0(\{\bar{\sigma}\},\{1\}) - E_0(\{\sigma_\alpha'^z\},\{\tau_\alpha\})]} \tag{4.2}$$

when neither $\{\sigma_\alpha^z\}$ nor $\{\sigma_\alpha'^z\}$ equals $\{\bar{\sigma}\}$, and

$$\frac{\langle \{\bar{\sigma}\} \mid H_1' \mid \{\sigma_\alpha'^z\} \rangle}{E_0'(\{\bar{\sigma}\}) - E_0'(\{\sigma_\alpha'^z\})} + \frac{\langle \{\bar{\sigma}\} \mid H_2' \mid \{\sigma_\alpha'^z\} \rangle}{E_0'(\{\bar{\sigma}\}) - E_0'(\{\sigma_\alpha'^z\})} + \sum_{\substack{\{\sigma_\alpha''^z\} \\ E_0'(\{\sigma_\alpha''^z\}) \neq E_0'(\{\bar{\sigma}\})}} \frac{\langle \{\bar{\sigma}\} \mid H_1' \mid \{\sigma_\alpha''^z\} \rangle}{E_0'(\{\bar{\sigma}\}) - E_0'(\{\sigma_\alpha''^z\})} \frac{\langle \{\sigma_\alpha''^z\} \mid H_1' \mid \{\sigma_\alpha'^z\} \rangle}{E_0'(\{\bar{\sigma}\}) - E_0'(\{\sigma_\alpha'^z\})}$$

$$= \frac{\langle \{\bar{\sigma}\},\{1\} \mid V \mid \{\sigma_\alpha'^z\}.\{1\} \rangle}{E_0(\{\bar{\sigma}\},\{1\}) - E_0(\{\sigma_\alpha'^z\}),\{1\})}$$

$$+ \sum_{\substack{\{\sigma_\alpha''^z\},\{\tau_\alpha''\} \\ E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\}) \\ \neq E_0(\{\bar{\sigma}\},\{1\})}} \frac{\langle \{\bar{\sigma}\},\{1\} \mid V \mid \{\sigma_\alpha''^z\},\{\tau_\alpha''\} \rangle \langle \{\sigma_\alpha''^z\},\{\tau_\alpha''\} \mid V \mid \{\sigma_\alpha'^z\},\{1\} \rangle}{[E_0(\{\bar{\sigma}\},\{1\}) - E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\})][E_0(\{\bar{\sigma}\},\{1\}) - E_0(\{\sigma_\alpha'^z\},\{1\})]} \tag{4.3}$$

when $\{\sigma_\alpha^z\} = \{\bar{\sigma}\}$, $\{\sigma_\alpha'^z\} \neq \{\bar{\sigma}\}$, and

$$\tfrac{1}{2}\beta'^2 \mid \langle \{\bar{\sigma}\} \mid H_1' \mid \{\bar{\sigma}\} \rangle \mid^2 = \tfrac{1}{2}\beta^2 \mid \langle \{\bar{\sigma}\},\{1\} \mid V \{\bar{\sigma}\},\{1\} \rangle \mid^2 \tag{4.4}$$

when $\{\sigma_\alpha^z\} = \{\sigma_\alpha'^z = \{\bar{\sigma}\}$. The equation for the case $\{\sigma_\alpha^z\} \neq \{\bar{\sigma}\} = \{\sigma_\alpha'^z\}$ is, of course, analogous to (4.3). One can easily check that the first-order SLAC result for $\langle \{\sigma_\alpha^z\} \mid H_i' \mid \{\sigma_\alpha'^z\} \rangle$ is not compatible with (4.2), for example. In this sense the second-order $\beta \to \infty$ limit derivation cannot be seen as a perturbative extension of the limit in Sec. III.

The reason for this is simple: If we denote by $|0\rangle$ and E the perturbative ground state and its energy [$|0\rangle = |\{\bar{\sigma}\},\{1\}\rangle + \cdots$; $E = E_0(\{\bar{\sigma}\},\{1\}) + \cdots$], we have that, asymptotically for $\beta \to \infty$,

$$e^{-\beta H} \simeq e^{-\beta E} |0\rangle\langle 0| . \tag{4.5}$$

Consequently, in order to avoid the appearance of the exponential $\exp[-\beta E_0(\{\bar{\sigma}\},\{1\})]$ [$\simeq \exp(-\beta E)$] in (3.6), $\{\sigma_\alpha^z\}$ and $\sigma_\alpha'^z\}$ must satisfy the condition

$$\mathrm{Tr}_{\{\tau_\alpha\}}\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}\,|\,0\rangle\langle 0\,|\,\{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle=0\ . \tag{4.6}$$

With the first-order ground state, this condition is satisfied as soon as both $\{\sigma_\alpha^z\}$ and $\{\sigma_\alpha'^z\}$ are different from $\{\bar{\sigma}\}$. In second order instead, $|0\rangle$ has a structure such that (4.6) can never be satisfied. This essentially makes the determination of H' so different in the two cases.

The solution of the above difficulty is to modify the choice of the states $|\{\sigma_\alpha^z\},\{\tau_\alpha\}\rangle$ that enter in the definition of the transformation (3.6). One can actually proceed in two different ways.

The first procedure consists of trying to make the algorithm in first order look similar to the second-order one by a generic choice of $|\{\sigma_\alpha^z\},\{\tau_\alpha\}\rangle$ that does not satisfy (4.6) even in first order. One thus makes the whole situation analogous to that discussed in Sec. II, where we did not have such problems of consistency. In this way, however, one loses the limit result obtained in Sec. III. On the other hand, the SLAC transformation can, of course, be replaced by very efficient substitutes, as we will show in the next section.

The second possibility consists of performing a modification of the states that does not influence the first-order SLAC results. In this case one must try to make the second-order calculation as similar as possible to that of Sec. III, avoiding there also the appearance of exponentials more dominant than

$$\exp[-\beta E_0(\{\sigma_\alpha^z\},\{1\})]$$

or

$$\exp[-\beta E_0(\{\sigma_\alpha'^z\},\{1\})]\ .$$

In order to apply this technique, we can modify the definition of our free-energy–preserving mapping (3.6) in the following way:

$$\langle\{\sigma_\alpha^z\}\,|\,e^{-\beta' H'}\,|\,\{\sigma_\alpha'^z\}\rangle=\mathrm{Tr}_{\{\tau_\alpha\}}\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}\,|\,U^{-1}e^{-\beta H}U\,|\,\{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle\ , \tag{4.7}$$

where U is a unitary operator that has the effect of rotating the states $|\{\sigma_\alpha^z\},\{\tau_\alpha\}\rangle$. The unitary character of U of course guarantees the invariance of the free energy under the transformation.

Since our aim is that of maintaining the validity of the first-order results of Sec. III in the limit $\beta\to\infty$, we will try to use a U of the form

$$U=1+U_1+U_2+U_3+\cdots\ , \tag{4.8}$$

with the U_i being a correction of ith order in the intercell interaction V. There is, of course, still enormous freedom *a priori* in the choice of U. Our further requirement on U will be that, at least asymptotically in the limit $\beta\to\infty$, in a second-order expansion of (4.7), the new terms introduced by the presence of U itself should cancel exactly the unwanted terms with exponentials of energies below the minimum of $E_0(\{\sigma_\alpha^z\},\{1\})$ and $E_0(\{\sigma_\alpha'^z\},\{1\})$. Imposing such a requirement on U does not yet determine it completely, and the remaining freedom can be considered as pertaining to the definition of the renormalization transformation.

The construction of a U satisfying the above-mentioned requirements can be performed, in principle, up to any order in the intercell coupling. In Appendix B we work out a particular choice of U in second order, such that (4.7), in the $\beta\to\infty$ limit, exactly implies the transformation of Ref. 20, which is characterized by (4.1) for the renormalized H_2' matrix elements. With this choice it turns out that the transformed Hamiltonian $\beta' H'$ has a spectrum in perturbation theory that coincides with the low-lying part of the spectrum of βH for β going to infinity. The preservation of the low-lying part of the spectrum was the basic requirement for the definition of the transformation in Ref. 20. The basic requirement in finite-temperature renormalization calculations is the preservation of the free energy. In principle, this implies the preservation of the whole energy spectrum, since the canonical partition function is the Laplace transform of the energy density.

V. RECURSION METHOD OF FRIEDMAN AND SUBBARAO AND ITS FINITE-TEMPERATURE EXTENSION

In the preceding section we mentioned the possibility of drastically modifying the states $|\{\sigma_\alpha^z\},\{\tau_\alpha\}\rangle$, used in the derivation of the SLAC mapping, in order to avoid the problems encountered when passing from the limit of a first-order transformation to that of a second-order one. Here we will consider a particularly interesting and efficient alternative to the SLAC choice of states; this alternative choice forms the basis of the zero-temperature renormalization method first introduced by Friedman[10] and later improved and developed by Subbarao.[11]

To be specific, let us focus our attention again on the example of the Ising model in a transverse field, with a Hamiltonian of the form (3.1). Taking into account that the zero-temperature critical phenomenon in the model is due to long-range fluctua-

tions in the S^x components of the spins, it was suggested in Ref. 10 to define a renormalization transformation in which the eigenvalues of the cell spin components σ_α^x are made equal to those of the operator sign $(\sum_{i\in\alpha} S_i^x)$ for cells with an odd number of spins. Since this operator does not commute with the Hamiltonian (3.1), its eigenvectors clearly cannot also be cell energy eigenstates.

As was already noted by Friedman and Subbarao, their ground-state transformation must correspond to the zero-temperature limit of a general mapping defined by the equation

$$\langle\{\sigma_\alpha^x\}e^{-\beta' H'}\,|\,\{\sigma_\alpha'^x\}\rangle = \mathrm{Tr}_{\{\tau_\alpha\}}\langle\{\sigma_\alpha^x\},\{\tau_\alpha\}\,|\,e^{-\beta H}\,|\,\{\sigma_\alpha'^x\},\{\tau_\alpha\}\rangle\ , \tag{5.1}$$

where now the states $|\{\sigma_\alpha^x\},\{\tau_\alpha\}\rangle$ are direct products of cell states $|\sigma_\alpha^x,\tau_\alpha\rangle_\alpha$, given by

$$\begin{aligned}
|1,1\rangle_\alpha &= |+++\rangle_x\ ,\\
|-1,1\rangle_\alpha &= |---\rangle_x\ ,\\
|1,2\rangle_\alpha &= |-++\rangle_x\ ,\\
|-1,2\rangle_\alpha &= |+--\rangle_x\ ,\\
|1,3\rangle_\alpha &= |+-+\rangle_x\ ,\\
|-1,3\rangle_\alpha &= |-+-\rangle_x\ ,\\
|1,4\rangle_\alpha &= |++-\rangle_x\ ,\\
|-1,4\rangle_\alpha &= |--+\rangle_x\ .
\end{aligned} \tag{5.2}$$

Here $|\epsilon_1\epsilon_2\epsilon_3\rangle_x$ with $\epsilon_i=\pm1$ represents the cell spin state that is composed of the eigenvectors of S_i^x belonging to the eigenvalues ϵ_i. Equations (5.2) define what is called a "majority rule" for the cell spin component σ_α^x.[3]

It may be noted that (5.2) can be seen as a special realization of (4.7), where the unitary operator replaces the $\{\sigma_\alpha^z\}$ states by the $\{\sigma_\alpha^x\}$ states; according to (5.1) we have applied an analogous unitary operator to the lhs of (4.7). Such an operator is not of the perturbative type (4.8), but it corresponds to the first procedure for modifying the states $|\{\sigma_\alpha^z\},\{\tau_\alpha\}\rangle$, as mentioned in the preceding section.

In Refs. 10 and 11 no attempt was made to compute (5.1) for finite temperature, and only the zero-temperature realization of the transformation was carried out, making use of the asymptotic property (4.5) for $e^{\beta H}$ and $e^{\beta' H'}$. In the previous sections, on the other hand, we showed that the $\beta\to\infty$ limit of a transformation such as (5.1), computed up to a given order in V with our expansion scheme (2.11), can lead to the same results as those obtained at zero temperature by Rayleigh-Schrödinger perturbation theory in V to the same order. It is thus meaningful and consistent to extrapolate down to vanishingly small temperatures the transformation computed in our finite-temperature approximation. We are able to show that, for the mapping defined by (5.1), the $\beta\to\infty$ limit leads, order by order, to the perturbative results of Refs. 10 and 11. This is shown in detail in Appendix C of this paper.

The finite-temperature extensions of the calculations of Refs. 10 and 11 obtained in this way are extremely important and useful, since this approach is seriously limited as long as one cannot treat the finite-temperature case. Indeed, in Refs. 10 and 11 the z exponent could not be computed, but had to be introduced as an external piece of information in the setting up of the transformation. This impossibility of computing z is related to the fact that at zero temperature there is only one basic dimensionless coupling in the system, namely $x=\Gamma/J$.[35] Allowing instead for finite β's, we immediately introduce the extra dimensionless temperature parameter $T=(\beta J)^{-1}$. As we have seen in Sec. III, a transformation acting on these two parameters as represented by (3.15) allows us also to define the z exponent at the zero-temperature fixed point.

In the case of the transformation (5.1) up to first order the expression we obtain is of the same type as (3.14)–(3.17), with, however, a different R_1 function appearing in the definition of z and in the equation for the ground-state energy. The knowledge of the function R_1 immediately yields the z exponent, according to (3.17), and allows a consistent calculation of the ground-state energy by iteration of an equation of the form (2.9).

We have performed with our method test calculations of the z exponent and the ground-state energy for the linear and triangular Ising models in a transverse field. The values of our z exponents in $d=1$ and $d=2$ are reported in Table I, together with the ν and y_H exponents, and the fixed-point values x^*.[36] These values are computed from first-order transformations, involving linear and triangular three-spin cells for $d=1$ and $d=2$, respectively. These results are compared with the corresponding SLAC results, based on a three-spin cell in $d=1$ and on a four-spin cell in $d=2$. From this comparison one can see that the z exponent obtained with our finite-temperature extension of the approach of Refs. 10 and 11 is somewhat closer to the expected value than that in the SLAC case. A similar trend was already pointed out for the thermal exponent ν,

TABLE I. Results for the critical exponents ν, y_H, and z, and for the critical value x^* of $x=\Gamma/J$ of the transverse Ising model in $d=1$ and $d=2$ (triangular lattice). Our results, based on first-order finite-temperature extensions of the approach of Refs. 10 and 11, are compared with results obtained with the SLAC method (Refs. 14 and 15) and with the exact results (Ref. 37) or the results obtained from the series expansions on the $d=3$ classical Ising model. Our calculations are based on linear and triangular cells of three spins in $d=1$ and $d=2$, respectively. The SLAC results are obtained with the same cells in $d=1$, and with different four-spin cells in $d=2$.

	$d=1$			$d=2$		
	SLAC method	This paper	Exact	SLAC method	This paper	Series expansions
ν	1.32	1.12	1	1.54	0.97	0.63
y_H	1.49	1.37	1.875	1.82	1.68	2.5
z	0.63	0.73	1	0.33	0.63	1
x^*	1.155	1.009	1	4.118	3.319	

whereas a better value of the magnetic exponent y_H seems to be reproduced by the SLAC approach.

We also notice that our calculation of z allows one to determine critical indices such as α, the specific-heat exponent, in a fully consistent way without assuming the knowledge of the exact result for z. In the above cases it results that the α values obtained with our approximate z are somewhat better than those obtained by assuming $z=1$ ($\alpha=0.05$ instead of -0.25 for $d=2$, and $\alpha=-0.55$ instead of -0.95 in $d=3$; the exact and expected values should be 0 and 0.125, respectively).

As we already noted, our extension in temperature is also crucial for consistent calculations of the ground-state energy. In Ref. 11 the neglect of the function R_1 was remedied by replacing it with a constant, equal to the expected exact fixed-point value i.e., $R_1=l^{-z}=1/l$. In Fig. 5 we have plotted the exact one-dimensional ground-state energy as a function of $x=\Gamma/J$, together with the approximate values computed with $R_1=l^{-1}$ (Ref. 11) and with our self-consistent method in first order (three-spin cells). The plots show very eloquently the crucial role played by the introduction of the actual function R_1 in the determination of a satisfactory overall behavior of the energy. Particularly remarkable is the improvement we get in the region of values near $x=0$. Our ground-state energy values are essentially comparable in accuracy with the values obtained by the SLAC approach in similar conditions (three-spin cells).

In regard to the comparison between the SLAC approach and the method of the present section, the z exponent that we find confirms the tendency of the other "thermal" quantities (like ν and x^*) to be better approximated in this scheme, whereas the ground-state energy has almost the same accuracy. The lower accuracy of the SLAC method for thermal quantities is probably due to the very peculiar choice of states $|\{\sigma_\alpha^z\},\{\tau_\alpha\}\rangle$ as unperturbed energy eigenstates. With such a choice only the lowest two energy eigenstates of the cells enter in the determination of the zero-temperature recursion formula, whereas in the transformation of the present section all cell states are involved.

VI. CONCLUDING REMARKS

In the present paper we have shown the existence of a deep unity underlying renormalization approaches at finite temperatures and ground-state iteration procedures for lattice quantum systems. In

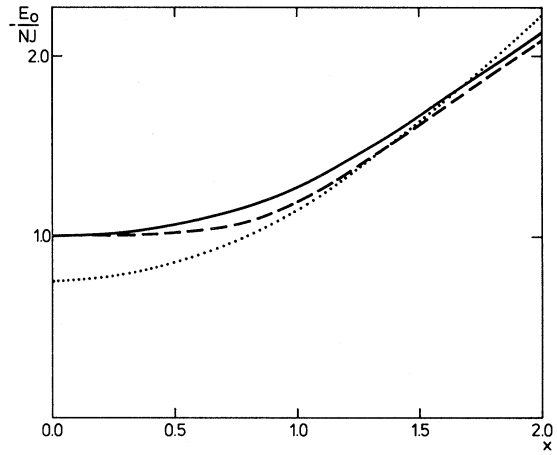

FIG. 5. Dimensionless ground-state energy density of the transverse Ising model, as a function of $x=\Gamma/J$ in $d=1$. Curves show the exact results from Ref. 37 (——), the results obtained by setting $R_1=l^{-1}$ as in Ref. 11 (· · ·), and the results of our self-consistent method (— — —).

all the cases considered, we indeed found that the ground-state approach can be seen as a zero-temperature limit of a free-energy–preserving mapping, induced by appropriate resummation conventions.

This general result has important conceptual and practical implications. First of all, contrary to a sort of widespread prejudice,[19] it reveals that the approximation schemes used for treating problems at finite temperature can give rise to meaningful zero-temperature extrapolations, that treat the ground-state problem as well as methods especially conceived for that purpose do.

A second important outcome of our derivations is the possibility of looking from a more unified perspective at the different zero-temperature techniques used in the current literature. In this respect we especially refer to the SLAC approach with its generalizations, and to the method of Refs. 10 and 11: These seemingly very different techniques can now be seen as corresponding to two alternative (and, to some extent, complementary) options within the same general scheme of renormalization at finite temperatures, as expressed by Eqs. (3.6) and (5.1).

The possibility of obtaining the z exponent in the SLAC method depends only on the fact that the approach can be formulated in terms of dimensional quantities, whereas the technique of Refs. 10 and 11 deals strictly with dimensionless quantities only. In the SLAC case, however, our extension is necessary if one wants to connect explicitly the exponent z with the scaling behavior of the system at extremely low temperatures. If we denote by $\tilde{\epsilon}$ the quantity f/K_1 (f being the dimensionless free-energy density), we have that close to the fixed point ($x=x^*$, $T=K_1^{-1}=0$), our transformation implies

$$\tilde{\epsilon}_s(x-x^*,T)\simeq l^{-d-z}\tilde{\epsilon}_s((x-x^*)l^{1/\nu},Tl^z) \quad (6.1)$$

for the singular part $\tilde{\epsilon}_s$ of $\tilde{\epsilon}$. In the SLAC case, the corresponding scaling equation is merely

$$\epsilon_s(x-x^*)\simeq l^{-d-z}\epsilon_s((x-x^*)l^{1/\nu}) , \quad (6.2)$$

with the same ν and z, and with ϵ_s denoting the singular part of the ground-state energy density ϵ. Equations (6.1) and (6.2) are of course compatible, since we should have

$$\lim_{T\to 0}\tilde{\epsilon}(x,T)=\epsilon(x) . \quad (6.3)$$

In view of the large variety of applications that have been performed up to now, especially with the SLAC approach,[19] one can easily realize also that our extensions in temperature have a very wide and interesting range of potential applicability. With the few examples treated in the present paper we only intended to give an idea of some of the most interesting possibilities.

Our results for the triangular spin-$\frac{1}{2}$ XY model show that our renormalization technique is capable of yielding a consistent and satisfactory evaluation of the free energy of a system at all temperatures, from zero to infinity. Similar results had already been obtained for the one-dimensional case.[2] We are rather confident that our method could be extremely useful for a global investigation of the thermodynamics of fermion systems, like, e.g., the Hubbard model. For this model an appropriate version of the SLAC method has recently been proposed by Hirsch.[38,39] This approach seems to be rather promising, especially for the Hubbard chain.[40] A sucessful extension of this approach to finite temperatures has been performed; the results are planned to be published elsewhere.

As mentioned in the Introduction, our results for the Ising model with transverse field form an example of the way in which one can obtain a complete and consistent description of a system undergoing a critical phenomenon at zero temperature. In our approximations we can indeed discuss the critical behavior of the system at all temperatures (e.g., we can easily compute the critical temperature T_c as a function of x, for every x); in particular, we have access to the crossover region around the zero-temperature critical fixed point. A very eloquent confirmation of such possibilities is given, e.g., by the fact that for the first time we could compute the z exponent for the approach of Refs. 10 and 11. For this approach, from the results obtained with the ground-state energy calculations, we also demonstrated the extreme importance of having explicit control on the temperature behavior of the transformation.

ACKNOWLEDGMENT

One of us (C.V.) would like to thank Interuniversitair Instituut voor Kernwetenschappen, Belgium for financial support.

APPENDIX A

In Sec. III we discussed how to extend the SLAC ground-state renormalization method to finite temperatures. An example of a system to which this can be applied is the transverse Ising model with Hamiltonian (3.1) on the triangular lattice. Making the standard choice of triangular cells on this lattice,[3] one can easily calculate the eigenstates of the Hamiltonian H_0, restricted to the interior of a single cell. Our choice for the labeling of these states $|\sigma,\tau\rangle$ and for their relative phase factors is as follows:

$$
\begin{aligned}
&|+,1\rangle = C(1,1)[\,|+++\rangle + D(1,1)(\,|--+\rangle + |-+-\rangle + |+--\rangle)]\,,\\
&|+,2\rangle = \frac{1}{\sqrt{2}}(\,|++-\rangle - |-++\rangle)\,,\\
&|+,3\rangle = \frac{\sqrt{2}}{\sqrt{3}}\left[-\frac{1}{2}(\,|++-\rangle + |-++\rangle) + |+-+\rangle\right],\\
&|+,4\rangle = C(-1,1)[\,|+++\rangle + D(-1,1)(\,|--+\rangle + |-+-\rangle + |+--\rangle)]\,,\\
&|-,1\rangle = C(1,-1)[\,|---\rangle + D(1,-1)(\,|++-\rangle + |+-+\rangle + |-++\rangle)]\,,\\
&|-,2\rangle = -\frac{1}{\sqrt{2}}(\,|--+\rangle - |+--\rangle)\,,\\
&|-,3\rangle = \frac{\sqrt{2}}{\sqrt{3}}\left[\frac{1}{2}(\,|--+\rangle + |+--\rangle) - |-+-\rangle\right],\\
&|-,4\rangle = -C(-1,-1)[\,|---\rangle + D(-1,-1)(\,|++-\rangle + |+-+\rangle + |-++\rangle]\,,
\end{aligned}
\tag{A1}
$$

where, for $\epsilon=\pm1$ and $\sigma=\pm1$, and with $x=\Gamma/J$ as before, we have defined

$$C(\epsilon,\sigma)=[1+3D^2(\epsilon,\sigma)]^{-1/2}\,, \tag{A2a}$$

$$D(\epsilon,\sigma)=\tfrac{1}{3}A(\epsilon,\sigma)-\sigma x\,, \tag{A2b}$$

$$A(\epsilon,\sigma)=1+\sigma x+2\epsilon(1-\sigma x+x^2)^{1/2}\,. \tag{A2c}$$

The energies of these states are given by

$$
\begin{aligned}
&E_0(\sigma,1)=-JA(1,\sigma)\,,\\
&E_0(1,2)=E_0(1,3)=J-\Gamma\,,\\
&E_0(-1,2)=E_0(-1,3)=J+\Gamma\,,\\
&E_0(\sigma,4)=-JA(-1,\sigma)\,.
\end{aligned}
\tag{A3}
$$

It is tacitly understood that the signs in the spin states of (A1) refer to the z components of the cell spin or site spin operators.

The reason why we have chosen the relative phase factors of the states in this particular way lies in the fact that, in the limit $\Gamma\to0$, (A1) corresponds to the Niemeijer–van Leeuwen majority rule, insofar as the x components of the spin operators are concerned. In order to check this, we should perform the transformations

$$|\sigma,\tau\rangle_x=\frac{1}{\sqrt{2}}(\,|+,\tau\rangle_z+\sigma\,|-,\tau\rangle_z) \tag{A4}$$

on the cell spin states and analogous transformations on the site spin states on the rhs of (A1). In this way, it can be seen that the choice (A1) is equivalent (for $\Gamma=0$) to

$$
\begin{aligned}
&|+,1\rangle_x=|+++\rangle_x\,,\\
&|+,2\rangle_x=\frac{1}{\sqrt{2}}(\,|-++\rangle_x-|++-\rangle_x)\,,\\
&|+,3\rangle_x=\frac{1}{\sqrt{6}}(\,|-++\rangle_x-2\,|+-+\rangle_x+|++-\rangle_x)\,,\\
&|+,4\rangle_x=\frac{1}{\sqrt{3}}(\,|-++\rangle_x+|+-+\rangle_x+|++-\rangle_x)\,,\\
&|-,1\rangle_x=|---\rangle_x\,,\\
&|-,2\rangle_x=\frac{1}{\sqrt{2}}(\,|--+\rangle_x-|+--\rangle_x)\,,\\
&|-,3\rangle_x=-\frac{1}{\sqrt{6}}(\,|+--\rangle_x-2\,|-+-\rangle_x+|--+\rangle_x)\,,\\
&|-,4\rangle_x=\frac{1}{\sqrt{3}}(\,|+--\rangle_x+|-+-\rangle_x+|--+\rangle_x)\,.
\end{aligned}
\tag{A5}
$$

A different choice for the phase factors in (A1) would have led to a situation in which at least some of the

states with $\sigma_\alpha^x > 0$ would not have been built entirely from states with sign $\sum_{i\epsilon\alpha} S_i^x > 0$. Such a procedure could not lead to the Niemeijer–van Leeuwen result in the limit $\Gamma \to 0$.

APPENDIX B

In this appendix we want to show how a transformation, as defined in Eqs. (4.7) and (4.8), with a suitable choice of the unitary operator U can lead in the limit $\beta \to \infty$ to the transformation (4.1). Evaluating the rhs of (3.6), we get, in second order

$$\tfrac{1}{2}\beta^2 \sum_{\{\tau_\alpha\}} \sum_{\{\sigma_\alpha''^z\}} \sum_{\{\tau_\alpha''\}} \langle \{\sigma_\alpha^z\},\{\tau_\alpha\} \mid V \mid \{\sigma_\alpha''^z\},\{\tau_\alpha''\}\rangle \langle \{\sigma_\alpha''^z\},\{\tau_\alpha''\} \mid V \mid \{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle e^{-\beta E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\})}$$
$$\times \Omega_2(\beta E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\}) - \beta E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\}), \beta E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\}) - \beta E_0(\{\sigma_\alpha'^z\},\{\tau_\alpha\})) \tag{B1}$$

with

$$\Omega_2(x,y) = \frac{1}{2xy}\left[2 - (e^x + e^y) + \frac{y+x}{y-x}(e^y - e^x)\right] . \tag{B2}$$

Note that Ω_2 is symmetrical $[\Omega_2(x,y) = \Omega_2(y,x)]$ and had the following limiting values:

$$\Omega_2(0,x) = \lim_{y\to 0} \Omega_2(y,x) = \Omega(-x) = \Omega_2(x,0) , \tag{B3a}$$

$$\Omega_2(x,x) = \lim_{y\to x} \Omega_2(x,y) = e^x \Omega(x) , \tag{B3b}$$

$$\Omega_2(0,0) = \lim_{x\to 0} e^x \Omega(x) = \tfrac{1}{2} , \tag{B3c}$$

where $\Omega(x)$ was defined in (2.13).

Expression (B1), together with an analogous expansion on the lhs of (3.6), leads in the $\beta \to \infty$ limit to the awkward equations (4.2)–(4.4). We will show how it is possible to determine perturbatively a unitary operator

$$U = 1 + U_1 + U_2 + \cdots \tag{B4}$$

in order to compensate for the singular terms that appear in the expansion. Obviously, we have

$$U^\dagger = U^{-1} = 1 - U_1 - (U_2 - U_1^2) + \cdots . \tag{B5}$$

Inserting these operators in (4.7), we obtain in first order, besides the terms reproduced in (3.7), the following extra terms:

$$\sum_{\{\tau_\alpha\}} (e^{-\beta E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})} - e^{-\beta E_0(\{\sigma_\alpha'^z\},\{\tau_\alpha\})}) \times \langle \{\sigma_\alpha^z\},\{\tau_\alpha\} \mid U_1 \mid \{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle . \tag{B6}$$

In the limit $\beta \to \infty$ only the matrix element $\langle \{\sigma_\alpha^z\},\{1\} \mid U_1 \mid \{\sigma_\alpha'^z\},\{1\}\rangle$ survives and we must choose to set this equal to zero in order not to lose the first-order SLAC limit. Consequently,

$$\langle \{\sigma_\alpha^z\},\{1\} \mid U_1 \mid \{\sigma_\alpha'^z\},\{1\}\rangle = 0 . \tag{B7}$$

In second order, (4.7) yields the following extra terms, besides those appearing in (B1):

$$\sum_{\{\tau_\alpha\}} \Bigg[(e^{-\beta E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})} - e^{-\beta E_0(\{\sigma_\alpha'^z\},\{\tau_\alpha\})}) \langle \{\sigma_\alpha^z\},\{\tau_\alpha\} \mid U_2 \mid \{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle$$
$$+ \sum_{\{\sigma_\alpha''^z\}} \sum_{\{\tau_\alpha''\}} \langle \{\sigma_\alpha^z\},\{\tau_\alpha\} \mid U_1 \mid \{\sigma_\alpha''^z\},\{\tau_\alpha''\}\rangle \langle \{\sigma_\alpha''^z\},\{\tau_\alpha''\} \mid U_1 \mid \{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle$$
$$\times (e^{-\beta E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})} - e^{-\beta E_0(\{\sigma''^z_\alpha\},\{\tau_\alpha''\})})$$
$$+ \sum_{\{\sigma_\alpha''^z\}} \sum_{\{\tau_\alpha''\}} \beta \langle \{\sigma_\alpha^z\},\{\tau_\alpha\} \mid U_1 \mid \{\sigma_\alpha''^z\},\{\tau_\alpha''\},\rangle \langle \{\sigma_\alpha''^z\},\{\tau_\alpha''\} \mid V \mid \{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle$$
$$\times e^{-\beta E_0(\{\sigma_\alpha'^z\},\{\tau_\alpha\})} \chi(-\beta E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\}) + \beta E_0(\{\sigma_\alpha'^z\},\{\tau_\alpha\}))$$
$$- \sum_{\{\sigma_\alpha''^z\}} \sum_{\{\tau_\alpha''\}} \beta \langle \{\sigma_\alpha^z\},\{\tau_\alpha\} \mid V \mid \{\sigma_\alpha''^z\},\{\tau_\alpha''\}\rangle \langle \{\sigma_\alpha''^z\},\{\tau_\alpha''\} \mid U_1 \mid \{\sigma_\alpha'^z\},\{\tau_\alpha\}\rangle$$
$$\times e^{-\beta E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})} \chi(-\beta E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\}) + \beta E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})) \Bigg] , \tag{B8}$$

where $\chi(x)$ was defined in (3.8).

The sum of (B1) and (B8) corresponds to the full second-order contribution in the rhs of (4.7). This sum must be equated to the second-order part of the lhs of (4.7), which is of a form similar to (B1). From this identification, we can see that we obtain the result (4.1) in the limit $\beta\to\infty$ if we make the following choice for U [in combination with (B7)]:

$$\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}\,|\,U_1\,|\,\{\sigma_\alpha''^z\},\{\tau_\alpha''\}\rangle=\frac{\langle\{\sigma_\alpha^z\},\{\tau_\alpha\}\,|\,V\,|\,\{\sigma_\alpha''^z\},\{\tau_\alpha''\}\rangle}{E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\})-E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})}\ , \tag{B9a}$$

$$\langle\{\sigma_\alpha^z\},\{1\}\,|\,U_2\,|\,\{\sigma_\alpha'^z\},\{1\}\rangle=-\tfrac{1}{2}\langle\{\sigma_\alpha^z\},\{1\}\,|\,U_1^2\,|\,\{\sigma_\alpha'^z\},\{1\}\rangle\ . \tag{B9b}$$

Actually, in order to obtain (4.1), it is not necessary to impose (B9a) for all matrix elements of U_1, but only for those elements for which either $E_0(\{\sigma_\alpha^z\},\{\tau_\alpha\})$ or $E_0(\{\sigma_\alpha''^z\},\{\tau_\alpha''\})$ is lower than or equal to the maximum of $E_0(\{\sigma_\alpha^z\},\{1\})$ over all possible choices of $\{\sigma_\alpha^z\}$. The remaining matrix elements could, in principle, be choosen arbitrarily, since they are irrelevant to the ground-state mapping in second-order perturbation.

APPENDIX C

Here we show the equivalence between the ground-state method proposed by Friedman[10] and Subbarao[11] and the $\beta\to\infty$ limit of a procedure as defined in (5.1). In particular, we have to prove that, perturbatively in V,

$$\lim_{\beta\to\infty}[e^{\beta E}\langle\{\sigma_\alpha^x\},\{\tau_\alpha\}\,|\,e^{-\beta H}\,|\,\{\sigma_\alpha'^x\},\{\tau_\alpha\}\rangle]=\langle\{\sigma_\alpha^x\},\{\tau_\alpha\}\,|\,P(H)\,|\,\{\sigma_\alpha'^x\},\{\tau_\alpha\}\rangle\ , \tag{C1}$$

where E is the ground-state energy of the system, and $P(H)$ is the ground-state projector. Denoting by $X(\beta)_\infty$ the asymptotically dominating part of any function $X(\beta)$ when $\beta\to\infty$, such that

$$\lim_{\beta\to\infty}\frac{X(\beta)}{X(\beta)_\infty}=1\ , \tag{C2}$$

our aim will be to demonstrate that

$$\langle\{\sigma_\alpha^x\},\{\tau_\alpha\}\,|\,e^{-\beta H}\,|\,\{\sigma_\alpha'^x\},\{\tau_\alpha\}\rangle_\infty=[e^{-\beta E}\langle\{\sigma_\alpha^x\},\{\tau_\alpha\}\,|\,P(H)\,|\,\{\sigma_\alpha'^x\},\{\tau_\alpha\}\rangle]_\infty\ . \tag{C3}$$

This can be shown by expanding both sides perturbatively in V, where we use the Feynman identity (2.11) for the lhs and Rayleigh-Schrödinger perturbation theory for the rhs.

Since the states $|\{\sigma_\alpha^x\},\{\tau_\alpha\}\rangle$ are not eigenstates of H_0, we will denote the eigenstates of H_0 by $|n\rangle$ and their energies by E_0^n. In particular, in this appendix $|0\rangle$ and E_0^0 are the ground state of H_0 and its energy. Developing up to second order for the rhs of (C3), we obtain

$$\begin{aligned}e^{-\beta E}P(H)=e^{-\beta E_0^0}\Bigg[&\left[1-\sum_m{}'\frac{|\langle 0|V|m\rangle|^2}{E_0^0-E_0^m}\right]|0\rangle\langle 0|+\sum_n{}'\frac{\langle 0|V|n\rangle}{E_0^0-E_0^n}|0\rangle\langle n|+\sum_n{}'\frac{\langle n|V|0\rangle}{E_0^0-E_n^0}|n\rangle\langle 0|\\&+\sum_n{}'\sum_m{}'\left[\frac{\langle n|V|m\rangle\langle m|V|0\rangle}{(E_0^0-E_0^n)(E_0^0-E_0^m)}|n\rangle\langle 0|+\frac{\langle 0|V|m\rangle\langle m|V|n\rangle}{(E_0^0-E_0^n)(E_0^0-E_0^m)}|0\rangle\langle n|\right.\\&\left.+\frac{\langle n|V|0\rangle\langle 0|V|m\rangle}{(E_0^0-E_0^n)(E_0^0-E_0^m)}|n\rangle\langle m|\right]\\&-\sum_m{}'\left|\frac{\langle m|V|0\rangle}{E_0^0-E_0^m}\right|^2|0\rangle\langle 0|+\cdots\Bigg]\ .\end{aligned} \tag{C4}$$

$\sum'$ indicates a summation over all states, except the ground state. We have assumed that $\langle 0|V|0\rangle=0$, which is not a limitation of the method, since it can always be achieved by adding a constant term to H_0.

Every state $|\{\sigma_\alpha^x\},\{\tau_\alpha\}\rangle$ can be written as a linear combination of the eigenstates $|n\rangle$ of H_0:

$$|\{\sigma_\alpha^x\},\{\tau_\alpha\}\rangle=\sum_n C_{n\sigma\tau}|n\rangle\ , \tag{C5a}$$

with

$$C_{n\sigma\tau}=\langle n\,|\,\{\sigma_\alpha^x\},\{\tau_\alpha\}\rangle\ . \tag{C5b}$$

Using (C4) up to, e.g., first order in V, we obtain for the rhs of (C3):

$$[e^{-\beta E}\langle\{\sigma_\alpha^x\},\{\tau_\alpha\}\,|\,P(H)\,|\,\{\sigma_\alpha'^x\},\{\tau_\alpha\}\rangle]_\infty$$
$$=e^{-\beta E_0^0}\left[C_{0\sigma\tau}^* C_{0\sigma'\tau}+\sum_n{}'\left[\frac{\langle 0\,|\,V\,|\,n\rangle}{E_0^0-E_0^n}C_{0\sigma\tau}^* C_{n\sigma'\tau}+\frac{\langle n\,|\,V\,|\,0\rangle}{E_0^0-E_0^n}C_{n\sigma\tau}^* C_{0\sigma'\tau}\right]+\cdots\right]. \quad \text{(C6)}$$

Up to first order in V, the lhs of (C3) becomes with the aid of (2.11)

$$\left[\langle\{\sigma_\alpha^x\},\{\tau_\alpha\}\,|\,e^{-\beta H_0}\left[1-\int_0^\beta d\lambda\, e^{\lambda H_0}Ve^{-\lambda H_0}\right]\,|\,\{\sigma_\alpha'^x\},\{\tau_\alpha\}\rangle\right]_\infty$$
$$=\left[\sum_{n,m}C_{n\sigma\tau}^* C_{m\sigma'\tau}\left\langle n\left|e^{-\beta H_0}-e^{-\beta H_0}\int_0^\beta d\lambda\, e^{\lambda H_0}Ve^{-\lambda H_0}\right|m\right\rangle\right]_\infty$$
$$=\left[\sum_n C_{n\sigma\tau}^* C_{n\sigma'\tau}e^{-\beta E_0^n}-\sum_{nm}C_{n\sigma\tau}^* C_{m\sigma'\tau}\langle n\,|\,V\,|\,m\rangle e^{-\beta E_0^n}\chi(\beta E_0^n-\beta E_0^m)\right]_\infty, \quad \text{(C7)}$$

where we used definition (3.8). In this form, it is now simple to verify that (C6) and (C7) are equivalent. The same argument may be repeated for every order in V.

[1]J. A. Hertz, Phys. Rev. B 14, 1165 (1976).

[2]A. L. Stella, C. Vanderzande, and R. Dekeyser, Physica (Utrecht) 108B, 1065 (1981). Some of the results presented in the present paper were already reported here.

[3]Th. Niemeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1976), Vol. 6.

[4]J. Rogiers and R. Dekeyser, Phys. Rev. B 13, 4886 (1976).

[5]D. D. Betts and M. Plischke, Can. J. Phys. 54, 1553 (1976).

[6]A. L. Stella and F. Toigo, Physica (Utrecht) 89A, 175 (1977).

[7]R. C. Brower, F. Kuttner, M. Nauenberg, and K. Subbarao, Phys. Rev. Lett. 38, 1231 (1977).

[8]A. L. Stella and F. Toigo, Phys. Rev. B 17, 2343 (1978).

[9]R. Dekeyser, M. Reynaert, A. L. Stella, and F. Toigo, Phys. Rev. B 18, 3486 (1978).

[10]Z. Friedman, Phys. Rev. Lett. 36, 1326 (1976).

[11]K. Subbarao, Phys. Rev. Lett. 37, 1712 (1976).

[12]S. D. Drell, M. Weinstein, and S. Yankielowicz, Phys. Rev. D 14, 487 (1976); 16, 1769 (1977).

[13]R. Jullien, J. N. Fields, and S. Doniach, Phys. Rev. Lett. 38, 1500 (1977).

[14]R. Jullien, P. Pfeuty, J. N. Fields, and S. Doniach, Phys. Rev. B 18, 3568 (1978).

[15]K. A. Penson, R. Jullien, and P. Pfeuty, Phys. Rev. B 19, 4653 (1979).

[16]H. P. Van den Braak, W. J. Caspers, C. De Lange, and W. H. Willemse, Physica (Utrecht) 87A, 354 (1977).

[17]R. Dekeyser, J. Phys. (Paris) Colloq. C6, 747 (1978).

[18]W. J. Caspers, Phys. Rep. 63, 223 (1980). This review contains more extensive references on the approach of Refs. 16 and 18.

[19]R. Jullien, Can. J. Phys. 59, 605 (1981). This review article contains extensive references on the approach of Refs. 12–15.

[20]J. E. Hirsch and G. F. Mazenko, Phys. Rev. B 19, 2656 (1979).

[21]J. M. Rabin, Phys. Rev. B 21, 2027 (1980).

[22]L. G. Marland and D. D. Betts, Phys. Lett. 76A, 271 (1980).

[23]M. Suzuki and S. Miyashita, Can. J. Phys. 56, 902 (1978).

[24]D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic, New York, 1964).

[25]The number of interactions $J_1, J_2, \ldots$ to be considered in order to make the identification increases with increasing order in perturbation theory. In first order only J_1 is involved.

[26]M. Nauenberg and B. Nienhuis, Phys. Rev. Lett. 33, 1598 (1974).

[27]S. Katsura, Phys. Rev. 127, 1508 (1962).

[28]J. C. Bonner and M. E. Fisher, Phys. Rev. 135, 640 (1964).

[29]J. Rogiers, E. W. Grundke, and D. D. Betts, Can. J. Phys. 57, 1719 (1979).

[30]J. Rogiers, Can. J. Phys. 60, 368 (1982).

[31]In Ref. 17 this instability was erroneously reported as a divergence of the iteration (2.9) of the ground-state energy for the second-order transformation.

[32]J. Rogiers, T. Lookman, and D. D. Betts, Can. J. Phys. 56, 409 (1978).

[33]K. G. Wilson, Rev. Mod. Phys. 47, 1773 (1975).

[34]S. Jafarey, R. Pearson, D. J. Scalapino, and B. Stoeckley (unpublished).

[35]If we do not switch on an external field h in the x direc-

tion.

[36]The exponent y_H is defined by

$$y_H = \frac{1}{\ln l}\left[\ln \frac{\partial h'}{\partial h}\bigg|_{x^*, T=0, h=0}\right],$$

with h representing a dimensionless field in the x direction in spin space.

[37]P. Pfeuty, Ann. Phys. (N.Y.) 57, 79 (1970).
[38]J. Hirsch, Phys. Rev. B 22, 5259 (1980).
[39]C. Dasgupta and P. Pfeuty, J. Phys. C 14, 717 (1981).
[40]E. H. Lieb and F. Y. Wu, Phys. Rev Lett. 20, 1445 (1968).