

THE DETERMINATION OF THE GROUND-STATE ENERGY OF AN ANTIFERROMAGNETIC LATTICE BY MEANS OF A RENORMALIZATION PROCEDURE

H.P. VAN DE BRAAK, W.J. CASPERS, C. DE LANGE and M.W.M. WILLEMSE

Twente University of Technology, Enschede, The Netherlands

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An approximate value for the ground-state energy of an antiferromagnetic lattice of spins one-half is determined by means of a repeated renormalization procedure in which the lattice is divided into cells with an effective interaction. This effective interaction is determined on the basis of the spin-hamiltonian formalism.

1. Introduction

In the last decades the determination of the ground-state energy of an antiferromagnetic lattice has been the subject of a large number of theoretical calculations based on models consisting of lattices of spins one-half with an interaction of the well-known Heisenberg type, isotropic or anisotropic. So far exact results are only known for the linear chain¹⁾.

In the present work an approximate value for the ground-state energy per spin is determined by means of a repeated renormalization procedure in which the lattice is divided into Kadanoff cells. The effective interaction between the cells is determined on the basis of the spin-hamiltonian formalism²⁾. The accuracy of the method depends on the size of the cells and on the order in which the spin hamiltonian is evaluated.

In section 2 the partitioning of the lattice into cells, according to Kadanoff's scaling theory³⁾ is considered, together with the determination of the corresponding spin hamiltonian. In all cases the cells contain an odd number of spins, the lowest level of one isolated cell thus corresponding with a Kramers doublet. The interaction between the cells in the ground state of the lattice can be described in terms of a spin hamiltonian for the effective-spin variables corresponding with this Kramers doublet of the different cells.

For a Heisenberg system this spin hamiltonian is of the form of a constant plus a term that is, in lowest order, bilinear in the effective-spin components of different cells. In higher order also terms of a higher degree appear. Taking our model hamiltonian for the antiferromagnetic lattice of a sufficiently

general form we arrive, for all possible cells and all possible orders of the spin hamiltonian, at a transformation of the original problem into a similar one. There is a change, however, in the relevant parameters of the hamiltonian and an additive constant will appear. Repeating this transformation, or renormalization³), we arrive at a series expansion for the ground-state energy of the lattice corresponding with the additive constants for the successive steps. It is possible to have a realistic hamiltonian in the first step by taking a number of constants in the general hamiltonian equal to zero.

In section 3 the scaling and the renormalization transformation are considered in more detail and the concept of a fixed point is introduced. Our method is applied in section 4 to the linear chain with nearest and next-nearest neighbour interactions. In section 5 we compare our results with those in the literature and make some concluding remarks.

2. Spin-hamiltonian formalism and Kadanoff scaling

The interaction in the spin lattice is given by a hamiltonian $H(\mathbf{S}_i; \gamma, \delta, \dots)$ that depends on the spin vectors \mathbf{S}_i of the different lattice points i , and on a number of parameters γ, δ, \dots . This hamiltonian has the translational symmetry of the lattice, but the interaction may be of a general anisotropic type. We only consider spin moments $S = \frac{1}{2}$. The lattices we have especially in mind are the linear chain, the square lattice, and the simple cubic lattice, with interaction constants that depend only on the distance and not on the direction of the lattice vector connecting the sites.

In the lattices we consider a partition into Kadanoff cells of an odd number of sites, corresponding with $2l + 1$ neighbouring spins in the one-dimensional case, squares of $(2l + 1)^2$ spins for the square lattice and cubes of $(2l + 1)^3$ spins for the cubic lattice³). For this partition the lowest level for one isolated cell is a Kramers doublet.

Now the hamiltonian H can be divided into a part H_0 , describing the internal interactions in the cells and the rest H' giving coupling between the cells. In our method the evaluation of the spin hamiltonian in terms of H' for the lowest degenerate state of H_0 is essential²). The spin-hamiltonian method, being essentially Rayleigh-Schrödinger perturbation theory for a degenerate level, gives an effective hamiltonian for the ground state. The lowest state of H_0 has a degeneracy $2^{N'}$, N' being the number of cells given by $N/(2l + 1)^d$, in which N is the total number of sites and d the dimension of the lattice.

The example we shall consider in detail in section 4 is the linear chain with isotropic interaction, the strength depending on the distance, for which

$$H = 4 \sum_i \sum_{j \geq 1} \gamma(j) \mathbf{S}_i \cdot \mathbf{S}_{i+j} \quad (1)$$

We shall give the analysis for the smallest possible cells, $l = 1$, and for this case the division of H takes the form

$$H = H_0 + H',$$

$$H_0 = 4 \sum_k [\gamma(1)(S_{3k-1} \cdot S_{3k} + S_{3k} \cdot S_{3k+1}) + \gamma(2)S_{3k-1} \cdot S_{3k+1}]. \quad (2)$$

In the general case the unperturbed eigenstates for the lowest level will be denoted by $|\Phi_0^{(p)}\rangle$, p numbering the different, degenerate states, and the excited states by $|\Phi_n\rangle$. The degeneracy of the last states need not be expressed in the notation, different n corresponding with different states. The equations for the unperturbed states are

$$(H_0 - W_0)|\Phi_0^{(p)}\rangle = 0, \quad (H_0 - E_n)|\Phi_n\rangle = 0, \quad (3)$$

and the equation for the perturbed ground state can be written in the form

$$(H_0 + H')|\Psi_0^{(p)}\rangle = \sum_q E_0^{(p)} \delta_{pq} |\Psi_0^{(q)}\rangle,$$

$$(E_0^{(p)} - W_0) \delta_{pq} = \sum_{k=1}^{\infty} W_{k,pq} \quad (4)$$

The Rayleigh-Schrödinger method⁴) for this degenerate case leads to a representation of the matrix $(E_0^{(p)} - W_0) \delta_{pq}$ as a matrix series in terms of H' , the secular problem being formulated as the diagonalization of this matrix series. Whereas we find invariant expressions for the terms of this series, the diagonalization depends on the number of terms taken into account.

Eqs. (4) are solved by iteration of the set

$$|\Psi_0^{(p)}\rangle = |\Phi_0^{(p)}\rangle + \frac{P}{W_0 - H_0} (H' - E_0^{(p)} + W_0) |\Psi_0^{(p)}\rangle,$$

$$(E_0^{(p)} - W_0) \delta_{pq} = \langle \Phi_0^{(p)} | H' | \Psi_0^{(q)} \rangle, \quad (5)$$

P being the projection operator, projecting off the unperturbed ground multiplet $|\Phi_0^{(p)}\rangle$.

The second-order solution of eq. (5), which will be used in this paper, is

$$(W_1 + W_2)_{,pq} = \langle \Phi_0^{(p)} | H' | \Phi_0^{(q)} \rangle + \langle \Phi_0^{(p)} | H' \frac{P}{W_0 - H_0} H' | \Phi_0^{(q)} \rangle. \quad (6)$$

The lowest eigenvalue of (6) added to W_0 gives us the ground-state energy of the spin lattice in second order of H' . The solution of (5) can also be given in higher order, resulting in all instances in an effective hamiltonian for the

manifold $|\Phi_0^{(p)}\rangle$, the so-called spin hamiltonian. This spin hamiltonian can be expressed in terms of Pauli operators for the lowest Kramers doublets of the different Kadanoff cells into which the spin lattice has been divided.

For the case that the original hamiltonian is of a sufficiently general form $H = H(\mathbf{S}_i; \gamma, \delta, \dots)$ the spin hamiltonian for the lattice of Kadanoff cells gives a reproduction with parameters $\gamma^{(1)}, \delta^{(1)}, \dots$, generally different from the original set γ, δ, \dots .

$$\begin{aligned} H^{(1)}(\mathbf{S}_i^{(1)}, \gamma^{(1)}, \delta^{(1)}, \dots) \\ = \varepsilon_0(\gamma, \delta, \dots)NI^{(1)} + c_0(\gamma, \delta, \dots)H(\mathbf{S}_i^{(1)}, \gamma^{(1)}, \delta^{(1)}, \dots), \end{aligned} \quad (7)$$

in which $I^{(1)}$ stands for the unit operator in the linear manifold $|\Phi_0^{(p)}\rangle$, and $\mathbf{S}_i^{(1)}$ is the effective spin for the lowest Kramers doublet of cell i_1 . Eq. (7) may define ε_0 and c_0 in a unique way as a consequence of the condition that $H^{(1)}$ reproduces H apart from a multiplicative and an additive constant. In our example [cf. eq. (2)] uniqueness is realized if we take $\gamma^{(1)} = \gamma^{(1)}(1) = 1$, etc. The factor N is introduced in eq. (7) to make the relevant energy ε_0 independent of the size of the lattice. The constants ε_0 and c_0 , as well as the new parameters $\gamma^{(1)}, \delta^{(1)}, \dots$, are functions of the original parameter set γ, δ, \dots , and the recipe given in (7) is an example of a renormalization procedure. Repeating this procedure s times we arrive at

$$\begin{aligned} H^{(s)}(\mathbf{S}_{i_s}^{(s)}, \gamma^{(s)}, \delta^{(s)}, \dots) \\ = \left[\varepsilon_0(\gamma, \delta, \dots) + \frac{c_0(\gamma, \delta, \dots)}{n} \varepsilon_0(\gamma^{(1)}, \delta^{(1)}, \dots) \right. \\ \left. + \frac{c_0(\gamma, \delta, \dots)c_0(\gamma^{(1)}, \delta^{(1)}, \dots)}{n^2} \varepsilon_0(\gamma^{(2)}, \delta^{(2)}, \dots) + \dots \right. \\ \left. + \frac{1}{n^{s-1}} \left(\prod_{t=0}^{s-2} c_0(\gamma^{(t)}, \delta^{(t)}, \dots) \right) \varepsilon_0(\gamma^{(s-1)}, \delta^{(s-1)}, \dots) \right] NI^{(s)} \\ + \prod_{t=0}^{s-1} c_0(\gamma^{(t)}, \delta^{(t)}, \dots) H(\mathbf{S}_{i_s}^{(s)}, \gamma^{(s)}, \delta^{(s)}, \dots), \\ \gamma^{(0)} = \gamma, \quad \delta^{(0)} = \delta, \dots, \quad n = (2l+1)^d. \end{aligned} \quad (8)$$

In (8) n is the number of spins per cell, N/n being the number of cells, or pseudospins, after the first renormalization, N/n^k after the k th, etc. . . . The corresponding set of parameters are $\gamma^{(1)}, \delta^{(1)}, \dots, \gamma^{(k)}, \delta^{(k)}, \dots$, etc. and $I^{(s)}$ is the unit operator for the pseudo-spin space after the s th renormalization. It stands to reason that N has to be a multiple of n^s for the procedure to be possible s times.

In the next section the scaling leading from a given space to one of a lower dimension according to the recipe given in eqs. (7) and (8) is considered in

more detail; the bracketed part of eq. (8) immediately gives a series expansion for the ground-state energy per spin.

3. Series expansion for the ground-state energy

Now the ground-state energy per spin in the limit ($N \rightarrow \infty$, $s \rightarrow \infty$) can be easily derived from (8) under the condition that only the bracketed part makes a contribution. That this is indeed the case may be readily demonstrated for the practical cases we have considered. In those cases the parameter set $(\gamma^{(s)}, \delta^{(s)}, \dots)$ converges to a unique fixed point, which gives us the possibility to evaluate the bounds for the energy per spin in terms of a geometrical series. In our numerical calculations we simply iterated the renormalization transformation and then added the corresponding contributions to the energy per spin until a sufficient accuracy was reached.

The renormalization transformation is given by a set of universal functions, i.e. functions independent of s

$$\gamma^{(s)} = \Gamma(\gamma^{(s-1)}, \delta^{(s-1)}, \dots), \quad \delta^{(s)} = \Delta(\gamma^{(s-1)}, \delta^{(s-1)}, \dots), \dots \quad (9)$$

A fixed point for such a transformation: $(\gamma^*, \delta^*, \dots)$, is defined by the equations³⁾

$$\gamma^* = \Gamma(\gamma^*, \delta^*, \dots), \quad \delta^* = \Delta(\gamma^*, \delta^*, \dots), \quad (10)$$

and it turns out that for all the practical cases we have considered there is only one fixed point and that the set $(\gamma^{(s)}, \delta^{(s)}, \dots)$ rapidly converges to this fixed point. This means that in these cases the parameters may be replaced by those corresponding with the fixed point after a reasonable number of scaling transformations or renormalizations.

On the basis of the foregoing we may write for the ground-state energy per spin

$$\begin{aligned} \varepsilon(\gamma, \delta, \dots) &= \varepsilon_0(\gamma, \delta, \dots) + \frac{c_0(\gamma, \delta, \dots)}{n} \varepsilon_0(\gamma^{(1)}, \delta^{(1)}, \dots) \\ &\quad + \frac{c_0(\gamma, \delta, \dots)c_0(\gamma^{(1)}, \delta^{(1)}, \dots)}{n^2} \varepsilon_0(\gamma^{(2)}, \delta^{(2)}, \dots) + \dots \\ &= \varepsilon_0(\gamma, \delta, \dots) + \sum_{s=1}^{\infty} \frac{1}{n^s} \left(\prod_{t=0}^{s-1} c_0(\gamma^{(t)}, \delta^{(t)}, \dots) \right) \varepsilon_0(\gamma^{(s)}, \delta^{(s)}, \dots), \quad (11) \end{aligned}$$

a formula that will be used for practical calculations. In the next section our method will be used in the case of a linear chain for which the spin hamiltonian will be evaluated in second order. The general formula for this approximation was given in (6).

4. An example: the linear chain

Formula (1) gives the general hamiltonian for the linear chain with isotropic interaction. In this section we restrict ourselves to the case $\gamma(j) = 0$ for $j > 2$, and normalize the energy in such a way that $\gamma(1) = 1$. The symbol $\gamma(2)$ will be replaced by γ . The zero-order hamiltonian, which for the general case was already given in (2), may now be written

$$H_0 = \sum_k H_{0,k},$$

$$H_{0,k} = 4(\mathbf{S}_{3k-1} \cdot \mathbf{S}_{3k} + \mathbf{S}_{3k} \cdot \mathbf{S}_{3k+1}) + 4\gamma \mathbf{S}_{3k-1} \cdot \mathbf{S}_{3k+1}, \quad (12)$$

for Kadanoff cells of three spins, $l = 1$. The explicit expression for H' reads

$$H' = \sum_k H'_{k,k+1},$$

$$H'_{k,k+1} = 4\mathbf{S}_{3k+1} \cdot \mathbf{S}_{3k+2} + 4\gamma(\mathbf{S}_{3k} \cdot \mathbf{S}_{3k+2} + \mathbf{S}_{3k+1} \cdot \mathbf{S}_{3k+3}). \quad (13)$$

Now our first task is to determine the eigenstates $|\Phi_0^{(p)}\rangle, |\Phi_n\rangle$ for this case, and the corresponding eigenvalues W_0, E_n . Because H_0 is a sum of terms corresponding to different cells, which are all identical, we simply have to determine the stationary states for one single cell. The total spin S for a cell is a good quantum number and there are two doublets ($S = \frac{1}{2}$) and one quartet ($S = \frac{3}{2}$) per cell. As a basis for cell k we take eigenstates of $\mathbf{S}_{3k-1,z}, \mathbf{S}_{3k,z}, \mathbf{S}_{3k+1,z}$, denoted by $|+++\rangle_k, |++-\rangle_k$, etc. . . . , the + or - denoting, respectively, up and down states for the three spins. In table I we have given the stationary states for one cell and the corresponding energy eigenvalue ϵ , omitting the index k .

The \pm sign in the symbols $|\frac{1}{2}\pm, m\rangle$ indicates the symmetry character for the interchange of the first and the last of the group of three spins. For $\gamma < 1$ the doublet $|\frac{1}{2}+, m\rangle$ corresponds to the lowest energy. Only for these values of γ will our perturbation series be considered. The doublet for the three spins $\mathbf{S}_{3k-1}, \mathbf{S}_{3k}, \mathbf{S}_{3k+1}$, i.e. the k th cell, corresponds to the effective spin $\mathbf{S}_{i_1}^{(1)}$ as introduced in formula (7) (the vector i stands for one of the numbers $3k-1, 3k, 3k+1$ and i_1 for k). The constant term in $H^{(1)}$ has a part of zero order: $\frac{1}{3}\epsilon_0(\gamma)NI^{(1)}$, $\epsilon_0(\gamma)$ being given in table I. Denoting the parts of zero, first and second order of $H^{(1)}$ by $H_0^{(1)}, H_1^{(1)}$ and $H_2^{(1)}$, respectively, we have

$$H_0^{(1)} = \frac{1}{3}(-4 + \gamma)NI^{(1)}. \quad (14)$$

For the first-order contribution we have to know the zero-order state vectors, but these are simply the eigenstates of the set $\mathbf{S}_{k,z}^{(1)}: \Pi_k |\frac{1}{2}+, m_k\rangle = |\dots m_{k-1}, m_k, m_{k+1} \dots\rangle$, denoted by $|\Phi_0^{(p)}\rangle$ in the general formula (6). For the first-order term to be calculated we have to determine the matrix elements

TABLE I
The stationary states for a cell of three spins

| | m | | $\epsilon(\gamma)$ |
|---------------------------|----------------|--|--------------------------------------|
| $ \frac{3}{2}, m\rangle$ | $\frac{3}{2}$ | $ +++ \rangle$ | } $2 + \gamma$ |
| | $\frac{1}{2}$ | $\frac{1}{\sqrt{3}} +-+\rangle + \frac{1}{\sqrt{3}}[-++\rangle + ++-\rangle]$ | |
| | $-\frac{1}{2}$ | $\frac{1}{\sqrt{3}} -+-\rangle + \frac{1}{\sqrt{3}}[+--\rangle + --+\rangle]$ | |
| | $-\frac{3}{2}$ | $ --- \rangle$ | |
| $ \frac{1}{2}, m\rangle$ | $\frac{1}{2}$ | $\frac{1}{\sqrt{2}}[-++\rangle - ++-\rangle]$ | } -3γ |
| | $-\frac{1}{2}$ | $-\frac{1}{\sqrt{2}}[+--\rangle - --+\rangle]$ | |
| $ \frac{1}{2}+, m\rangle$ | $\frac{1}{2}$ | $-\frac{2}{\sqrt{6}} +-+\rangle + \frac{1}{\sqrt{6}}[-++\rangle + ++-\rangle]$ | } $-4 + \gamma = \epsilon_0(\gamma)$ |
| | $-\frac{1}{2}$ | $\frac{2}{\sqrt{6}} -+-\rangle - \frac{1}{\sqrt{6}}[+--\rangle + --+\rangle]$ | |

$\langle \frac{1}{2}+, m_k | \mathbf{S}_{3k\pm 1} | \frac{1}{2}+, m_k \rangle$, $\langle \frac{1}{2}+, m_k | \mathbf{S}_{3k} | \frac{1}{2}+, m_k \rangle$, which can all be expressed in terms of $\mathbf{S}_k^{(1)}$, according to the Wigner-Eckart theorem⁵

$$\begin{aligned}
 \langle \frac{1}{2}+, m_k | \mathbf{S}_{3k} | \frac{1}{2}+, m_k \rangle &= -\frac{1}{3} \langle \frac{1}{2}+, m_k | \mathbf{S}_k^{(1)} | \frac{1}{2}+, m_k \rangle, \\
 \langle \frac{1}{2}+, m_k | \mathbf{S}_{3k\pm 1} | \frac{1}{2}+, m_k \rangle &= \frac{2}{3} \langle \frac{1}{2}+, m_k | \mathbf{S}_k^{(1)} | \frac{1}{2}+, m_k \rangle, \\
 \mathbf{S}_k^{(1)} &= P_{\frac{1}{2}+}(k)(\mathbf{S}_{3k-1} + \mathbf{S}_{3k} + \mathbf{S}_{3k+1})P_{\frac{1}{2}+}(k).
 \end{aligned}
 \tag{15}$$

The projection operator $P_{\frac{1}{2}+}(k)$ projects on the doublet $|\frac{1}{2}+, m_k\rangle$ for cell k . In eq. (15) only one numerical constant, e.g. $-\frac{1}{3}$ in the first line, had to be determined by explicit calculation of one matrix element.

On the basis of (15) the first-order part $H_1^{(1)}$ can now be calculated and it turns out that it has the simple form of a sum of scalar interaction terms for the spins $\mathbf{S}_k^{(1)}$ of neighbouring cells

$$H_1^{(1)} = \frac{16}{9}(1 - \gamma) \sum_k \mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+1}.
 \tag{16}$$

For the determination of the second order part of $H^{(1)}$ we have to know the form of the projection operator P that appears in the general expression for

this second-order contribution in (6):

$$\left\langle \Phi_0^{(p)} \left| H' \frac{P}{W_0 - H_0} H' \right| \Phi_0^{(q)} \right\rangle.$$

Careful inspection shows that, in this order, P may be replaced in our example by a sum of terms corresponding to the excitation of one cell or of two neighbouring cells. The projection operator $\bar{P}_{\frac{1}{2}}(k)$ will project on the ground state for all cells, with the exception of the k th cell, for which it is a projection on the doublet: $|\frac{1}{2}-, m_k\rangle$. The projection operator $\bar{P}_{\frac{3}{2}}$ is defined in an analogous way, whereas $\bar{P}_{\frac{1}{2}-\frac{1}{2}}(k, k+1)$ projects on a state in which two neighbouring cells are in the excited state $|\frac{1}{2}-, m\rangle$, etc. With these definitions we have

$$\begin{aligned} \frac{P}{W_0 - H_0} H' |\Phi_0^{(p)}\rangle &= \frac{P}{W_0 - H_0} H' \prod_k P_{\frac{1}{2}+}(k) |\Phi_0^{(p)}\rangle \\ &= \sum_k \left[\frac{1}{-4 + 4\gamma} \bar{P}_{\frac{1}{2}}(k) + \frac{1}{-6} \bar{P}_{\frac{3}{2}}(k) + \frac{1}{2(-4 + 4\gamma)} \bar{P}_{\frac{1}{2}-\frac{1}{2}}(k, k+1) \right. \\ &\quad + \frac{1}{-10 + 4\gamma} (\bar{P}_{\frac{1}{2}-\frac{3}{2}}(k, k+1) + \bar{P}_{\frac{3}{2}-\frac{1}{2}}(k, k+1)) \\ &\quad \left. + \frac{1}{2(-6)} \bar{P}_{\frac{3}{2}\frac{3}{2}}(k, k+1) \right] H' \prod_{k'} P_{\frac{1}{2}+}(k') |\Phi_0^{(p)}\rangle. \end{aligned} \tag{17}$$

Only the terms $H'_{k-1,k}$ and $H'_{k,k+1}$ in (13) may result in the excitation of the k th cell, whereas only $H'_{k,k+1}$ gives the double excitation of the neighbour pair $(k, k+1)$. In order to evaluate (17) we now give expressions for the projected operators $P_{\frac{1}{2}+}(k)S_{3k}P_{\frac{1}{2}+}(k)$, $P_{\frac{1}{2}+}(k)S_{3k\pm 1}P_{\frac{1}{2}+}(k)$, $P_{\frac{1}{2}-}(k)S_{3k}P_{\frac{1}{2}+}(k)$, etc. which can easily be derived if one makes use of the symmetry of the eigenstates in table I. The results are given in table II. Some of the results were already used in formula (15).

TABLE II
Projected operators for cell k

| | |
|-------------------------------------|---|
| $P_{1/2+}(k)S_{3k}P_{1/2+}(k)$ | $= -\frac{1}{3}(S_{3k-1} + S_{3k} + S_{3k+1})P_{1/2+}(k),$ |
| $P_{1/2+}(k)S_{3k\pm 1}P_{1/2+}(k)$ | $= \frac{2}{3}(S_{3k-1} + S_{3k} + S_{3k+1})P_{1/2+}(k),$ |
| $P_{1/2-}(k)S_{3k}P_{1/2+}(k)$ | $= 0,$ |
| $P_{1/2-}(k)S_{3k\pm 1}P_{1/2+}(k)$ | $= \pm\frac{1}{2}(-S_{3k-1} + S_{3k+1})P_{1/2+}(k),$ |
| $P_{3/2}(k)S_{3k}P_{1/2+}(k)$ | $= \frac{1}{3}(S_{3k-1} + 4S_{3k} + S_{3k+1})P_{1/2+}(k),$ |
| $P_{3/2}(k)S_{3k\pm 1}P_{1/2+}(k)$ | $= -\frac{1}{6}(S_{3k-1} + 4S_{3k} + S_{3k+1})P_{1/2+}(k).$ |

The effective operators in the right-hand members of table II are chosen in such a way that they connect the states $|\frac{1}{2}+, m\rangle$ only with the states $|\frac{1}{2}+, m'\rangle$,

$|\frac{1}{2}^-, m'\rangle$ and $|\frac{3}{2}^-, m'\rangle$, respectively, and for that reason there appears only one projection operator in these right-hand members. From table II the different projected parts of H' in the last member of eq. (17) may be evaluated in a straightforward way. They are given in table III.

TABLE III
Projected parts of H'

$$\begin{aligned} \bar{P}_{1/2^-, (k)} H' \prod_{k'} P_{1/2^-, (k')} &= \frac{2}{3}(2 - \gamma)(S_{3k-1} - S_{3k+1}) \cdot \{(S_{3k-4} + S_{3k-3} + S_{3k-2}) \\ &- (S_{3k+2} + S_{3k+3} + S_{3k+4})\} \prod_{k'} P_{1/2^+, (k')}, \\ \bar{P}_{3/2^-, (k)} H' \prod_{k'} P_{1/2^+, (k')} &= \frac{2}{9}(-2 + 5\gamma)(S_{3k-1} + 4S_{3k} + S_{3k+1}) \cdot \{(S_{3k-4} + S_{3k-3} \\ &+ S_{3k-2}) + (S_{3k+2} + S_{3k+3} + S_{3k+4})\} \prod_{k'} P_{1/2^-, (k')}, \\ \bar{P}_{1/2^-, 1/2^-, (k, k+1)} H' \prod_{k'} P_{1/2^+, (k')} &= -(S_{3k-1} - S_{3k+1}) \cdot (S_{3k+2} - S_{3k-4}) \prod_{k'} P_{1/2^+, (k')}, \\ \bar{P}_{1/2^-, 3/2^-, (k, k+1)} H' \prod_{k'} P_{1/2^+, (k')} &= \frac{1}{3}(1 - 2\gamma)(S_{3k-1} - S_{3k+1}) \cdot (S_{3k-2} \\ &+ 4S_{3k+3} + S_{3k+4}) \prod_{k'} P_{1/2^+, (k')}, \\ \bar{P}_{3/2^-, 1/2^-, (k, k+1)} H' \prod_{k'} P_{1/2^-, (k')} &= -\frac{1}{3}(1 - 2\gamma)(S_{3k-1} + 4S_{3k} + S_{3k+1}) \\ &\cdot (S_{3k+2} - S_{3k-4}) \prod_{k'} P_{1/2^+, (k')}, \\ \bar{P}_{3/2^-, 3/2^-, (k, k+1)} H' \prod_{k'} P_{1/2^+, (k')} &= \frac{1}{9}(1 - 4\gamma)(S_{3k-1} + 4S_{3k} + S_{3k+1}) \\ &\cdot (S_{3k+2} + 4S_{3k+3} + S_{3k+4}) \prod_{k'} P_{1/2^+, (k')}. \end{aligned}$$

The evaluation of the second-order part of (6) in our example results in the evaluations of the products

$$\prod_{k'} P_{\frac{1}{2}^+, (k')} H' \bar{P}_{\frac{1}{2}^-, (k)} \frac{1}{W_0 - H_0} \bar{P}_{\frac{1}{2}^-, (k)} H' \prod_{k''} P_{\frac{1}{2}^+, (k'')}, \quad \text{etc.}$$

which can be written with table III in terms of the spin operators of two neighbouring cells, or of two cells that are next neighbours. It will be demonstrated that our recipe gives a reproduction of the original hamiltonian, because the second-order contribution to $H^{(1)}$ can also be written in terms of the $S_k^{(1)}$, apart from a constant. For reasons of time-reversal symmetry and the spherical symmetry of the original hamiltonian (1) only bilinear terms of the

form $c\mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+1}^{(1)}$ and $d\mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+2}^{(1)}$ appear, hermitean forms quadratic in the components of one single spin $\mathbf{S}_k^{(1)}$ giving a constant.

In the calculations it is convenient to have simplified expressions for the dyads $P_{\frac{1}{2}+}(k)\mathbf{S}_{3k}\mathbf{S}_{3k}P_{\frac{1}{2}+}(k)$, $P_{\frac{1}{2}+}(k)\mathbf{S}_{3k}\mathbf{S}_{3k\pm 1}P_{\frac{1}{2}+}(k)$, etc. of the spin vectors of one cell in terms of the two dyads $\mathbf{S}_k^{(1)}\mathbf{S}_k^{(1)}$ and $\mathbf{1}$. The dyad $P_{\frac{1}{2}+}(k)\mathbf{S}_{3k}\mathbf{S}_{3k}P_{\frac{1}{2}+}(k)$, for instance, is a shorthand notation for the set $P_{\frac{1}{2}+}(k)\mathbf{S}_{3k,\xi}\mathbf{S}_{3k,\eta}P_{\frac{1}{2}+}(k)$, $\xi, \eta = x, y, z$, and the unit dyad $\mathbf{1}$ corresponds with the Kronecker delta. A complete set of effective dyadic forms is given in table IV.

TABLE IV
Effective dyadic forms for the k th cell.

| | |
|---|--|
| $P_{1/2-}(k)\mathbf{S}_{3k}\mathbf{S}_{3k}P_{1/2-}(k) =$ | $-\frac{1}{3}\mathbf{S}_k^{(1)}\mathbf{S}_k^{(1)} + \frac{1}{3}\mathbf{1}$ |
| $P_{1/2+}(k)\mathbf{S}_{3k}\mathbf{S}_{3k\pm 1}P_{1/2+}(k) = P_{1/2-}(k)\mathbf{S}_{3k\pm 1}\mathbf{S}_{3k}P_{1/2-}(k) =$ | $-\frac{1}{6}\mathbf{1}$ |
| $P_{1/2+}(k)\mathbf{S}_{3k\pm 1}\mathbf{S}_{3k\pm 1}P_{1/2+}(k) =$ | $\frac{2}{3}\mathbf{S}_k^{(1)}\mathbf{S}_k^{(1)} + \frac{1}{12}\mathbf{1}$ |
| $P_{1/2-}(k)\mathbf{S}_{3k+1}\mathbf{S}_{3k+1}P_{1/2-}(k) =$ | $\frac{1}{12}\mathbf{1}$ |

In the evaluation of the second-order part of $H^{(1)}$ there appear also terms of the form $(\mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+1}^{(1)})^2$. These terms may readily be reduced by means of the relation

$$(\mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+1}^{(1)})^2 = \frac{3}{16} - \frac{1}{2}(\mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+1}^{(1)}). \quad (18)$$

Making use of formulae (6), (17) and (18) and tables III and IV we find for the sum of all second-order terms

$$\begin{aligned} H_2^{(1)} = & \left[-\frac{3-16\gamma+22\gamma^2}{27} - \frac{19-16\gamma+4\gamma^2}{72(1-\gamma)} - \frac{2}{9} \frac{1-4\gamma+4\gamma^2}{5-2\gamma} \right] \frac{N}{3} I^{(1)} \\ & + \left[-\frac{2}{81} (5-24\gamma+28\gamma^2) + \frac{19-16\gamma+4\gamma^2}{27(1-\gamma)} \right. \\ & \quad \left. - \frac{8}{27} \frac{1-4\gamma+4\gamma^2}{5-2\gamma} \right] \sum_k \mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+1}^{(1)} \\ & + \left[-\frac{8}{243} (4-20\gamma+25\gamma^2) + \frac{2}{27} \frac{4-4\gamma+\gamma^2}{1-\gamma} \right] \sum_k \mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+2}^{(1)}. \end{aligned} \quad (19)$$

The sum of the three contributions $H_0^{(1)}$, $H_1^{(1)}$ and $H_2^{(1)}$, given in eqs. (14), (16) and (19), respectively, amounts to the spin hamiltonian of formula (7) up to and including the second order

$$\begin{aligned} H^{(1)} = & \left[-\frac{111-43\gamma+22\gamma^2}{27} - \frac{19-16\gamma+4\gamma^2}{72(1-\gamma)} - \frac{2}{9} \frac{1-4\gamma+4\gamma^2}{5-2\gamma} \right] \frac{N}{3} I^{(1)} \\ & + \left[\frac{2}{81} (67-48\gamma-28\gamma^2) + \frac{19-16\gamma+4\gamma^2}{27(1-\gamma)} - \frac{8}{27} \frac{1-4\gamma+4\gamma^2}{5-2\gamma} \right] \sum_k \mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+1}^{(1)} \end{aligned}$$

$$+ \left[-\frac{8}{243} (4 - 20\gamma + 25\gamma^2) + \frac{2}{27} \frac{4 - 4\gamma + \gamma^2}{1 - \gamma} \right] \sum_k \mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+2}^{(1)}. \quad (20)$$

With this expression for $H^{(1)}$ the functions $\varepsilon_0(\gamma)$, $c_0(\gamma)$ and $\gamma^{(1)} = \Gamma(\gamma)$, essential for the renormalization in our example, are given by

$$\begin{aligned} \varepsilon_0(\gamma) &= \frac{1}{3} \left[-\frac{111 - 43\gamma + 22\gamma^2}{27} - \frac{19 - 16\gamma + 4\gamma^2}{72(1 - \gamma)} - \frac{2}{9} \frac{1 - 4\gamma + 4\gamma^2}{5 - 2\gamma} \right], \\ c_0(\gamma) &= \frac{1}{4} \left[\frac{2}{81} (67 - 48\gamma - 28\gamma^2) + \frac{19 - 16\gamma + 4\gamma^2}{27(1 - \gamma)} - \frac{8}{27} \frac{1 - 4\gamma + 4\gamma^2}{5 - 2\gamma} \right], \\ \gamma^{(1)} = \Gamma(\gamma) &= \frac{1}{4c_0(\gamma)} \left[-\frac{8}{243} (4 - 20\gamma + 25\gamma^2) + \frac{2}{27} \frac{4 - 4\gamma + \gamma^2}{1 - \gamma} \right]. \end{aligned} \quad (21)$$

The definition of $\varepsilon_0(\gamma)$ and $c_0(\gamma)$ was given by formula (7). The γ values were defined by (1) and for our example we took $\gamma(1) = \gamma^{(1)}(1) = 1$ and $\gamma(2) = \gamma$, $\gamma^{(1)}(2) = \gamma^{(1)}$. At this stage it is necessary to remark that only through a suitable combination of the size of the cell and the order of $H^{(1)}$ can a reproduction of the hamiltonian with a finite number of parameters be obtained.

The last of the equations (21) gives a possible stable point γ^* of the renormalization transformation, γ^* being a solution of $\gamma = \Gamma(\gamma)$ or

$$336\gamma^5 - 1216\gamma^4 - 188\gamma^3 + 3006\gamma^2 - 2273\gamma + 200 = 0. \quad (22)$$

We have already remarked, at the beginning of section 4, that only for $\gamma < 1$ is the doublet $|\frac{1}{2}^+, m\rangle$ the lowest level for a cell. In our numerical calculations for the linear chain we restrict ourselves to the parameter values $|\gamma| < 1$, and in this interval (22) has only one solution

$$\gamma^* = 0.10146,$$

corresponding to the stable point of our renormalization transformation: in the interval $|\gamma| < 1$ the function $\Gamma(\gamma)$, which has been drawn in fig. 1, has a slope between 0 and 1, so a repeated renormalization procedure will give a series of $\gamma^{(s)}$ converging to γ^* .

Now we are able to determine ε from the series given in (11). There is only one set of parameters $(\gamma, \gamma^{(1)}, \gamma^{(2)}, \dots)$ and $n = 3$. Values for ε_0 and c_0 as a function of γ , as well as $\Gamma(\gamma)$ of fig. 1, were calculated with the Wang 500 desk calculator. The results for ε were found by successive approximation, also with the Wang 500, along the lines indicated at the beginning of section 3. These results can be found in table V and fig. 2. The series (11) shows rapid convergence and $\gamma^{(s)}$ reaches the value γ^* with sufficient accuracy after a reasonable number of steps.

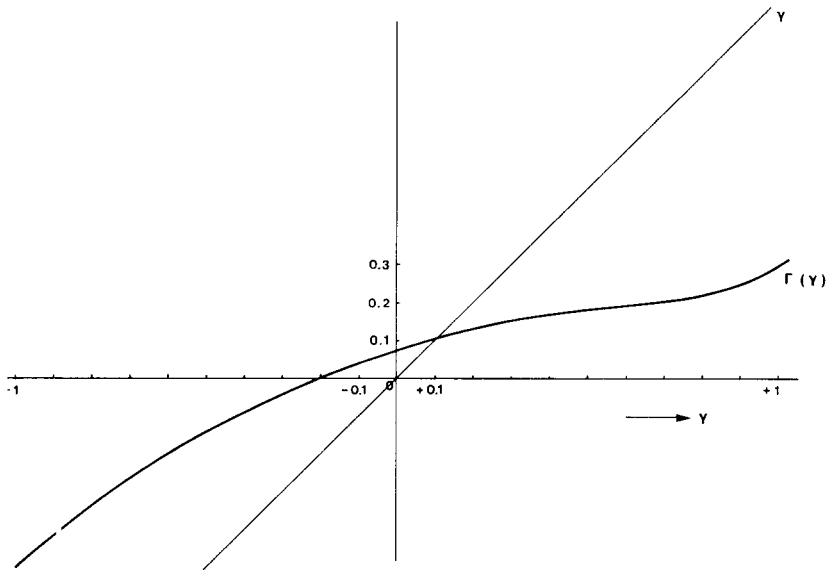


Fig. 1. The function $\Gamma(\gamma)$.

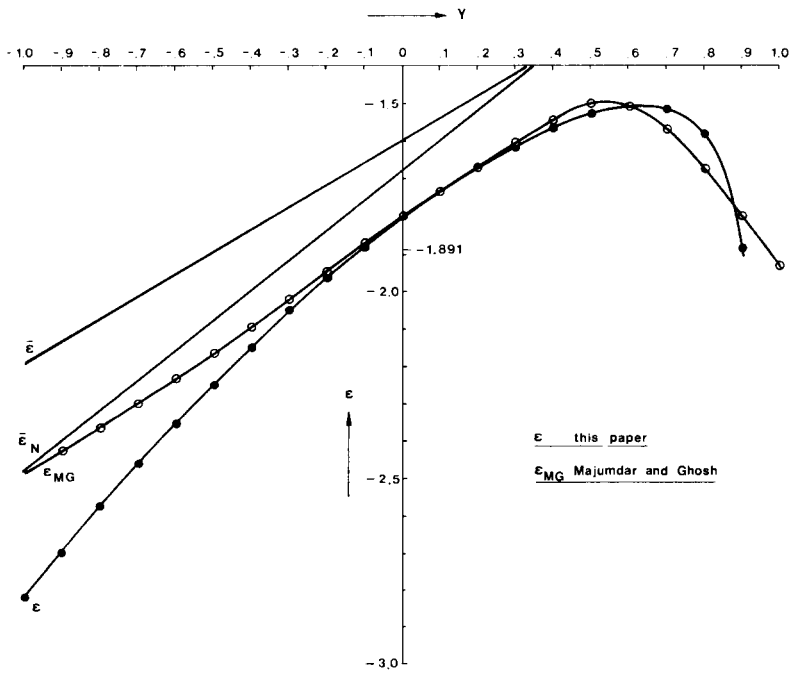


Fig. 2. Energy per spin for the linear chain.

TABLE V
 ε as a function of γ .

| γ | $-\varepsilon$ | γ | $-\varepsilon$ |
|----------|----------------|----------|----------------|
| -1 | 2.8281 | 0.1 | 1.7394 |
| -0.9 | 2.7010 | 0.2 | 1.6752 |
| -0.8 | 2.5798 | 0.3 | 1.6185 |
| -0.7 | 2.4644 | 0.4 | 1.5705 |
| -0.6 | 2.3545 | 0.5 | 1.5337 |
| -0.5 | 2.2501 | 0.6 | 1.5129 |
| -0.4 | 2.1511 | 0.65 | 1.5116 |
| -0.3 | 2.0575 | 0.7 | 1.5196 |
| -0.2 | 1.9694 | 0.8 | 1.5875 |
| -0.1 | 1.8868 | 0.9 | 1.8856 |
| 0 | 1.8101 | 0.95 | 2.5432 |

5. Concluding remarks

This work is concluded with a comparison of our results with those in the literature and by giving upper and lower bounds for $\varepsilon(\gamma)$. In fig. 2, apart from the results of this paper, we have also given the values for the energy per spin for a finite chain of ten particles computed by Majumdar and Ghosh⁷). The three values for $\varepsilon(0)$ computed by Hulthén⁶), Majumdar and Ghosh, and by us are in that order:

$$\varepsilon_{\text{H}}(0) = -1.7726, \quad \varepsilon_{\text{MG}}(0) = -1.8062 \quad \text{and} \quad \varepsilon(0) = -1.8101.$$

An upper bound for the whole range of γ values is found by determining $H^{(1)}$ in first order. This operator corresponds with the projection of H on the space of product states for the lattice of Kadanoff cells of three spins, all cells being in one of the states of their lowest Kramers doublet. From eqs. (14) and (16) it follows that in this approximation

$$H^{(1)} = \frac{1}{3}(-4 + \gamma)NI^{(1)} + \frac{16}{9}(1 - \gamma) \sum_k \mathbf{S}_k^{(1)} \cdot \mathbf{S}_{k+1}^{(1)}. \quad (23)$$

The lowest eigenvalue of $H^{(1)}$, per spin of the original lattice, immediately follows from Hulthén's result, so one finds the upper bound

$$\bar{\varepsilon} = \frac{1}{3}(-4 + \gamma) + \frac{16}{9}(1 - \gamma)^{\frac{1}{3}} \cdot \frac{1}{4} \cdot (-1.77258) = -1.5960 + 0.5960\gamma.$$

The upper bound given by Niemeijer⁸) equals

$$\bar{\varepsilon}_{\text{N}} = 4 \left(-\frac{1}{\pi} - \frac{1}{\pi^2} + \frac{2\gamma}{\pi^2} \right) = -1.6785 + 0.8106\gamma,$$

which gives, for relevant values of γ , a far better estimate. (For values of $\gamma \sim 1$ our approximation is very poor.) The upper bounds $\bar{\varepsilon}$ and $\bar{\varepsilon}_N$ are also drawn in fig. 2.

Fig. 2 finally shows a lower bound for $\gamma = 0$. This lower bound is calculated along the following lines. For $\gamma = 0$ we have, for the linear chain, an example of a Bravais lattice with only nearest-neighbour interaction. Other examples are the square and the cubic lattice, the interaction in which is also restricted to nearest neighbours. We suppose that in all three cases the ground state is nondegenerate and has the full symmetry of the antiferromagnetic lattice. Now every pair of neighbour spins contributes the same energy in this ground state. Again we consider a division of the lattice into Kadanoff cells and the corresponding partition of H , $H = H_0 + H'$, discussed in section 2, H' corresponding to the bonds between the cells. For an isolated cell the number of bonds equals

$$(2l + 1)^d \cdot d - \frac{1}{2}(2l + 1)^{d-1} \cdot 2d = (2l + 1)^{d-1} \cdot 2l,$$

the last term in the first member corresponding to the number of external bonds per cell. It is clear that the bonds between the cells contribute the fraction $1/(2l + 1)$ to the total energy of the ground state. Now the lowest eigenvalue of H may be written as the sum of the expectation values of H_0 and H' in the ground state, and for the first expectation value we have a lower bound, given by its lowest eigenvalue. So we may write the asymptotic formula

$$\langle H \rangle = N\varepsilon + o(N) = \langle H_0 \rangle + \langle H' \rangle \geq \frac{N\varepsilon_0}{(2l + 1)^d} + \frac{N\varepsilon}{2l + 1} + o(N). \quad (24)$$

in which ε_0 is the lowest eigenvalue of H_0 per cell. The symbol $o(N)$ denotes a term of vanishing order as compared to N . A lower bound for ε in terms of ε_0 immediately follows from (24):

$$\varepsilon \geq \frac{2l + 1}{2l} \frac{\varepsilon_0}{(2l + 1)^d}. \quad (25)$$

For our one-dimensional example ($d = 1$) with cells of three spins ($l = 1$), ε_0 is given in table I: $\varepsilon_0 = -4$ ($\gamma = 0$). So we find $\varepsilon \geq -2$.

This lower boundary serves as a mere illustration. A better value can be calculated by taking larger cells, e.g. $2l + 1 = 7$ for which we find a lowest eigenvalue per cell $\varepsilon_0 = -11.3450$ resulting in

$$\varepsilon \geq -\frac{1}{6}11.3450 = -1.891.$$

There is a wide range of possible applications of our formalism. We have

only given a simple example which clearly demonstrates the applicability of the approximation method.

At the conclusion of this work our attention was drawn to a paper by Friedman⁹) in which a similar renormalization transformation for a spin hamiltonian was introduced with a different purpose. For the triangular lattice with triangular cells Friedman introduces as an example, our method does not work because the lowest level of a cell in this case is not a Kramers doublet.

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