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Two-parameter expansions for quantum spin systems

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Abstract. As an extension of our one-parameter series expansion, a two-parameter expansion technique for quantum spin systems is developed. As examples of the method we present results for three different models on the square lattice: the (2+1)-dimensional Ising model with an external magnetic field, and the Heisenberg antiferromagnet with both an external staggered parallel magnetic field and an external perpendicular magnetic field. Analysis of the resulting series is also presented.

1. Introduction

There is currently a great deal of interest in quantum spin systems, such as the Heisenberg antiferromagnet, for many reasons, not least of which is the possible relevance to the mechanism of high-T_c superconductivity in the cuprates.

One important method for studying such systems is via long perturbation series, which can be most efficiently derived by the linked-cluster method, a technique first proposed by Nickel (1980), further elaborated by Marland (1981), and reviewed recently by He *et al* (1990). A very similar method seems to have been discovered independently by Singh and co-workers (Singh *et al* 1988, Gelfand *et al* 1990). During the past year we have successfully applied this method to study the Ising model (Oitmaa *et al* 1991), the Heisenberg antiferromagnet (Zheng *et al* 1991), the XY model (Hamer *et al* 1991), the three-state Potts model (Hamer *et al* 1992a), and the U(1) and SU(2) gauge models in 2+1 dimensions (Hamer *et al* 1992b).

In the present work we extend this technique to Hamiltonians which contain two perturbing terms and two parameters. Obvious candidate systems include antiferromagnets with further-neighbour interactions, where it has been suggested that frustration can lead to a new kind of ground state, a 'quantum spin liquid'. We intend to investigate such systems in further work. Here as illustrations of our technique, we apply it to three different models on the square lattice: the (2+1)-dimensional Ising model with an external magnetic field, the Heisenberg antiferromagnet with an external staggered parallel magnetic field and the Heisenberg antiferromagnet with an external perpendicular magnetic field. The analysis of the resulting series is also presented.

The plan of this paper is as follows: in section 2 the theory of the two-parameter expansion is reviewed, the applications are presented in section 3 and section 4 is devoted to a summary and discussion.

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2. Theory

We consider a lattice Hamiltonian of the form:

$$H = H_0 + xV_1 + yV_2 \tag{1}$$

and choose a basis in which H_0 is diagonal with ground-state energy $E_{0,0}$ and eigenvector $|\psi_{0,0}\rangle$. The terms V_1 and V_2 are to be treated as perturbations, with x and y as the expansion parameters.

We seek to expand the ground state $|\Psi_0\rangle$ of H and its corresponding energy E_0 in the form

$$|\Psi_0\rangle = \sum_{i,j=0} x^i y^j |\psi_{i,j}\rangle \tag{2}$$

$$E_0 = \sum_{i,j=0} E_{i,j} x^i y^j . \tag{3}$$

If we also want to calculate other ground-state properties, such as the magnetization and susceptibility, we need to include an extra term zV_3 representing the magnetic field interaction, so the full Hamiltonian becomes

$$H = H_0 + xV_1 + yV_2 + zV_3. \tag{4}$$

The expansion in z is usually needed to order z^2, so we can formally expand the ground state $|\Psi_0\rangle$ and its energy E_0 for the above Hamiltonian in the following form:

$$|\Psi_0\rangle = \sum_{i,j=0} x^i y^j (|\psi_{i,j}\rangle + z|\psi'_{i,j}\rangle + \tfrac{1}{2}z^2|\psi''_{i,j}\rangle + \cdots) \tag{5}$$

$$E_0 = \sum_{i,j=0} x^i y^j (E_{i,j} + zE'_{i,j} + \tfrac{1}{2}z^2 E''_{i,j} + \cdots). \tag{6}$$

The magnetization M and susceptibility χ are then

$$M = \sum_{i,j=0} E'_{i,j} x^i y^j \qquad \chi = -\sum_{i,j=0} E''_{i,j} x^i y^j . \tag{7}$$

By substituting (5) and (6) into the eigenvalue equation

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle \tag{8}$$

we get the following recurrence relations for $|\psi_{i,j}\rangle$, $|\psi'_{i,j}\rangle$ and $|\psi''_{i,j}\rangle$:

$$(H_0 - E_{0,0})|\psi_{i,j}\rangle = \sum_{k,l=0}^{i,j}{}' E_{i-k,j-l}|\psi_{k,l}\rangle - V_1|\psi_{i-1,j}\rangle - V_2|\psi_{i,j-1}\rangle \tag{9}$$

$$\begin{aligned}(H_0 - E_{0,0})|\psi'_{i,j}\rangle = {} & \sum_{k,l=0}^{i,j}{}' E_{i-k,j-l}|\psi'_{k,l}\rangle + \sum_{k,l=0}^{i,j} E'_{i-k,j-l}|\psi_{k,l}\rangle \\ & + (E'_{0,0} - V_3)|\psi_{i,j}\rangle - V_1|\psi'_{i-1,j}\rangle - V_2|\psi'_{i,j-1}\rangle\end{aligned} \tag{10}$$

$$\begin{aligned}(H_0 - E_{0,0})|\psi''_{i,j}\rangle = {} & \sum_{k,l=0}^{i,j}{}' E_{i-k,j-l}|\psi''_{k,l}\rangle + \sum_{k,l=0}^{i,j} (2E'_{i-k,j-l}|\psi'_{k,l}\rangle + E''_{i-k,j-l}|\psi_{k,l}\rangle) \\ & + 2(E'_{0,0} - V_3)|\psi'_{i,j}\rangle + E''_{0,0}|\psi_{i,j}\rangle - V_1|\psi''_{i-1,j}\rangle - V_2|\psi''_{i,j-1}\rangle\end{aligned} \tag{11}$$

where $\sum_{k,l=0}^{\prime i,j}$ means a sum over $k = 0,1,\ldots,i$, and $l = 0,1,\ldots,j$ except the case of $k = i$ and $l = j$ simultaneously. The initial conditions for above recurrence relations are

$$\begin{aligned} E'_{0,0} &= \langle\psi_{0,0}|V_3|\psi_{0,0}\rangle/\langle\psi_{0,0}|\psi_{0,0}\rangle \\ (H_0 - E_{0,0})|\psi'_{0,0}\rangle &= E'_{0,0}|\psi_{0,0}\rangle - V_3|\psi_{0,0}\rangle \\ E''_{0,0} &= 2\langle\psi_{0,0}|(V_3 - E'_{0,0})|\psi'_{0,0}\rangle/\langle\psi_{0,0}|\psi_{0,0}\rangle \\ (H_0 - E_{0,0})|\psi''_{0,0}\rangle &= 2(E'_{0,0} - V_3)|\psi'_{0,0}\rangle + E''_{0,0}|\psi_{0,0}\rangle. \end{aligned} \tag{12}$$

If we have complete knowledge of the ground state $|\Psi_0\rangle$ up to order (i,j), that is, $|\psi_{k,l}\rangle$, $|\psi'_{k,l}\rangle$ and $|\psi''_{k,l}\rangle$ ($k = 0,1,\ldots,i$, and $l = 0,1,\ldots,j$), we can define

$$|\Psi_0(i,j)\rangle = |\Psi_{i,j}\rangle + z|\Psi'_{i,j}\rangle + \tfrac{1}{2}z^2|\Psi''_{i,j}\rangle + \cdots \tag{13}$$

where

$$|\Psi_{i,j}\rangle = \sum_{k,l=0}^{i,j} x^k y^l |\psi_{k,l}\rangle \quad |\Psi'_{i,j}\rangle = \sum_{k,l=0}^{i,j} x^k y^l |\psi'_{k,l}\rangle \quad |\Psi''_{i,j}\rangle = \sum_{k,l=0}^{i,j} x^k y^l |\psi''_{k,l}\rangle. \tag{14}$$

Then

$$\langle\Psi_0(i,j)|\Psi_0(i,j)\rangle = Q_{i,j} + zQ'_{i,j} + \tfrac{1}{2}z^2 Q''_{i,j} + \mathrm{O}(z^3) \tag{15}$$

$$\langle\Psi_0(i,j)|(H_0 + xV_1 + yV_2)|\Psi_0(i,j)\rangle = P_{i,j} + zP'_{i,j} + \tfrac{1}{2}z^2 P''_{i,j} + \mathrm{O}(z^3) \tag{16}$$

where

$$\begin{aligned} Q_{i,j} &= \langle\Psi_{i,j}|\Psi_{i,j}\rangle \\ Q'_{i,j} &= \langle\Psi_{i,j}|\Psi'_{i,j}\rangle + \langle\Psi'_{i,j}|\Psi_{i,j}\rangle \\ Q''_{i,j} &= \langle\Psi_{i,j}|\Psi''_{i,j}\rangle + \langle\Psi''_{i,j}|\Psi_{i,j}\rangle + 2\langle\Psi'_{i,j}|\Psi'_{i,j}\rangle \end{aligned} \tag{17}$$

$$\begin{aligned} P_{i,j} &= \langle\Psi_{i,j}|H_0 + xV_1 + yV_2|\Psi_{i,j}\rangle \\ P'_{i,j} &= \langle\Psi'_{i,j}|H_0 + xV_1 + yV_2|\Psi_{i,j}\rangle + \langle\Psi_{i,j}|H_0 + xV_1 + yV_2|\Psi'_{i,j}\rangle + \langle\Psi_{i,j}|V_3|\Psi_{i,j}\rangle \\ P''_{i,j} &= \langle\Psi''_{i,j}|H_0 + xV_1 + yV_2|\Psi_{i,j}\rangle + \langle\Psi_{i,j}|H_0 + xV_1 + yV_2|\Psi''_{i,j}\rangle \\ &\quad + 2\langle\Psi'_{i,j}|H_0 + xV_1 + yV_2|\Psi'_{i,j}\rangle + 2\langle\Psi'_{i,j}|V_3|\Psi_{i,j}\rangle + 2\langle\Psi_{i,j}|V_3|\Psi'_{i,j}\rangle. \end{aligned} \tag{18}$$

It can be shown that a knowledge of the ground-state eigenvector up to order (i,j) is sufficient to derive the ground-state energy terms $E_{k,l}$, $E'_{k,l}$ and $E''_{k,l}$ up to order $(i, 2j+1)$ and $(2i+1, j)$ (denote these orders as A). These quantities $E_{k,l}$,

$E'_{k,l}$ and $E''_{k,l}$ can be obtained by comparing the coefficients of $x^k y^l$ in the following equations:

$$P_{i,j} = Q_{i,j} \sum_{A} E_{k,l} x^k y^l$$

$$P'_{i,j} = \sum_{A} (Q'_{i,j} E_{k,l} + Q_{i,j} E'_{k,l}) x^k y^l \tag{19}$$

$$P''_{i,j} = \sum_{A} (Q''_{i,j} E_{k,l} + Q_{i,j} E''_{k,l} + 2Q'_{i,j} E'_{k,l}) x^k y^l .$$

As with our previous work with one-parameter expansions, to proceed with the derivation of series by this method it is necessary to have the following data:

(a) a list of all clusters which give contributions to the series, up to the order required;

(b) the embedding constants of the clusters for the lattice under consideration;

(c) for each cluster, a list of subclusters and corresponding embedding constants.

We have developed an efficient algorithm for generating the above data. These have been reviewed by He *et al* (1990), and will not be repeated here.

3. Applications

We present here some preliminary results, using as test cases the following quantum spin systems on the square lattice.

3.1. (2+1)D Ising model with an external magnetic field

The system can be described by the following Hamiltonian:

$$H = \tfrac{1}{4} \sum_{\langle ij \rangle} (1 - \sigma_i^z \sigma_j^z) + \lambda \sum_i \sigma_i^x + \frac{y}{2} \sum_i \sigma_i^z \tag{20}$$

where the σ_i^α are Pauli spin operators acting on a two-state spin variable at site i of the lattice, $\langle ij \rangle$ denotes nearest-neighbour pairs, λ corresponds to the temperature in the Euclidean formulation and y is the magnetic field variable. We treat the first term of H as the unperturbed Hamiltonian, and the second and third terms as perturbations. The resulting series for the ground-state energy $E_0 = \sum E_{m,n} x^m y^n$ (where $x = \lambda^2$) is listed in table 1. The calculations involve a list of all linked clusters of up to 12 sites, together with their low-temperature (strong) lattice constants and data on their subclusters. This list of 3289 clusters was obtained previously in our study of the (2+1)D Ising model in zero external field (Oitmaa *et al* 1991). This information can be supplied on request.

The series can then be expressed in two ways.

Table 1. Series coefficients for the ground-state energy per site E_0 of Ising model with external magnetic field. Coefficients of $x^m y^n$ are listed ($x = \lambda^2$).

m	$E_{m,0}$	$E_{m,1}$	$E_{m,2}$	$E_{m,3}$
0	−0.000000000000E + 0	−5.000000000000E − 1	−0.000000000000E + 0	0.000000000000E + 0
1	−5.000000000000E − 1	2.500000000000E − 1	−1.250000000000E − 1	6.250000000000E − 2
2	−4.166666666667E − 2	1.736111111111E − 1	−3.032407407407E − 1	3.792438271605E − 1
3	−1.041666666667E − 2	1.467013888889E − 1	−5.423177083333E − 1	1.230426552855E + 0
4	−1.309317129630E − 2	2.022858796296E − 1	−1.112306435667E + 0	3.727450222774E + 0
5	−5.578579121656E − 3	2.250832953559E − 1	−1.937596508148E + 0	9.284051504241E + 0
6	−1.078810144599E − 2	3.481680145249E − 1	−3.734077675746E + 0	2.295316498583E + 1
7	−4.475800845599E − 3	4.168506552038E − 1	−6.335092932229E + 0	5.066441968399E + 1
8	−1.494260185289E − 2	7.194408081879E − 1	−1.212151474150E + 1	1.148699255974E + 2
9	−5.372145505638E − 3	8.958967252956E − 1	−2.048224941347E + 1	2.398005897024E + 2
10	−2.052255294622E − 2	1.538030379293E + 0	−3.786158505468E + 1	5.086802408954E + 2
11	−1.371351223876E − 2	2.151144545166E + 0	−6.570471585129E + 1	1.036830551780E + 3
12	−2.859105512001E − 2	3.467380088354E + 0	−1.174786762172E + 2	2.103841913273E + 3

m	$E_{m,4}$	$E_{m,5}$	$E_{m,6}$	$E_{m,7}$
0	0.000000000000E + 0	0.000000000000E + 0	0.000000000000E + 0	0.000000000000E + 0
1	−3.125000000000E − 2	1.562500000000E − 2	−7.812500000000E − 3	3.906250000000E − 3
2	−3.960583847737E − 1	3.695076731824E − 1	−3.192551154550E − 1	2.610138269700E − 1
3	−2.125165272151E + 0	3.074841032303E + 0	−3.927150400142E + 0	4.572212627686E + 0
4	−9.234462408221E + 0	1.861897303426E + 1	−3.231163552375E + 1	5.002890366101E + 1
5	−3.146996396564E + 1	8.428492463816E + 1	−1.899495398233E + 2	3.749810945893E + 2
6	−9.920667557473E + 1	3.347528513646E + 2	−9.387070339326E + 2	2.279074465283E + 3
7	−2.757928869746E + 2	1.149614157788E + 3	−3.926273445379E + 3	1.147731093578E + 4
8	−7.472809927322E + 2	3.710718440273E + 3	−1.500481435446E + 4	5.158422914301E + 4
9	−1.872326590014E + 3	1.099575763206E + 4	−5.206384503210E + 4	2.079435413737E + 5
10	−4.595671398120E + 3	3.116928069219E + 4	−1.697015478242E + 5	7.756022590964E + 5
11	−1.082602862560E + 4	8.414595010324E + 4	−5.218180854791E + 5	2.702550368264E + 6
12	−2.493401656350E + 4	2.192337452555E + 5	−1.531866385121E + 6	8.904246761313E + 6

m	$E_{m,8}$	$E_{m,9}$	$E_{m,10}$	$E_{m,11}$
0	0.000000000000E + 0	0.000000000000E + 0	0.000000000000E + 0	0.000000000000E + 0
1	−1.953125000000E − 3	9.765625000000E − 4	−4.882812500000E − 4	2.441406250000E − 4
2	−2.047709367300E − 1	1.556383067783E − 1	−1.153962409772E − 1	8.388883513064E − 2
3	−4.957144420152E + 0	5.080141536067E + 0	−4.974906213507E + 0	4.693693340919E + 0
4	−7.083262710832E + 1	9.334467041799E + 1	−1.160218420097E + 2	1.374093537163E + 2
5	−6.665617239910E + 2	1.088394069168E + 3	−1.657094407125E + 3	2.379888548946E + 3
6	−4.930099464497E + 3	9.703742890178E + 3	−1.765761057280E + 4	3.007747827033E + 4
7	−2.960211732695E + 4	6.887814793598E + 4	−1.470455046923E + 5	2.918596092356E + 5
8	−1.554409370877E + 5	4.199382251996E + 5	−1.034891174457E + 6	2.358382495796E + 6
9	−7.231288035628E + 5	2.241294288540E + 6	−6.303302223456E + 6	1.631354892338E + 7
10	−3.071664076658E + 6	1.079294832629E + 7	−3.426329085903E + 7	9.969740428092E + 7
11	−1.207350746500E + 7	4.765667728803E + 7	−1.693068360588E + 8	5.493460746603E + 8
12	−4.447904988124E + 7	1.956216913801E + 8	−7.718000234150E + 8	2.772465702225E + 9

3.1.1. x grouping. We write

$$E_0 = \sum_m e_m(y) x^m \tag{21}$$

where the $e_m(y)$ are available as power series through e_{12} from the horizontal sequences in table 1. In fact, it is simple to identify closed form expressions for $e_m(y)$, at least for small m, as

$$e_0(y) = -y/2 \tag{22a}$$

$$e_1(y) = -\frac{1}{y+2} \tag{22b}$$

$$e_2(y) = \frac{2y-1}{(y+2)^3\,(2y+3)} \tag{22c}$$

$$e_3(y) = \frac{-2\,(6-57y-20y^2+12y^3)}{(y+2)^5\,(2y+3)^2\,(3y+4)} \tag{22d}$$

$$e_4(y) = (-3620 + 24\,072\,y + 55\,055\,y^2 + 3313\,y^3 - 53\,738\,y^4 - 34\,172\,y^5 - 3144\,y^6 + 1440\,y^7)/[(y+2)^7\,(y+1)(2y+3)^3\,(3y+4)^2\,(4y+5)]. \tag{22e}$$

These results can also be obtained by combining the first and third terms in (20) as the unperturbed Hamiltonian with $V = \lambda \sum_i \sigma_i^x$ as the perturbation. Thus $e_m(y)$ will have poles at values of y corresponding to energy differences between unperturbed states.

3.1.2. y grouping. We write

$$E_0 = \sum_n \mathcal{E}_n(x) y^n. \tag{23}$$

The series $\mathcal{E}_0(x)$, $\mathcal{E}_1(x)$, $\mathcal{E}_2(x)$ are respectively the ground-state energy, magnetization, and susceptibility in zero field, which agree with our previous results (Oitmaa *et al* 1991). The other $\mathcal{E}_n(x)$ are series for higher field derivatives:

$$\mathcal{E}_n(x) = \lim_{y\to 0} \frac{1}{n!}\left(\frac{\partial^n E_0}{\partial y^n}\right). \tag{24}$$

Scaling theory (Stanley 1971) predicts that these should all diverge at the physical critical point, according to

$$\mathcal{E}_n \sim (x_c - x)^{-\alpha_n} \tag{25}$$

with $\alpha_n = \gamma + (n-2)\Delta$, where Δ is the gap exponent, which for the three-dimensional Ising model in the Euclidean formulation is $\Delta = 1.563(3)$ (Essam and Hunter 1968). Our previous estimate for x_c (He *et al* 1990, Oitmaa *et al* 1991) is $x_c \simeq 0.579\,1\bar{7}(14)$.

We have analysed the series for $\mathcal{E}_n(x)$ $(n \geqslant 3)$ by standard Dlog Padé approximants (Guttmann 1989). The analysis indicates that $\mathcal{E}_n(x)$ has a zero near the origin on the negative real x axis (i.e. imaginary λ)

$$\mathcal{E}_n(x) = (x_n^* - x)\overline{\mathcal{E}}_n(x) \tag{26}$$

and this zero completely masks the physical singularity. In table 2 we give our estimates of the position of this zero for different n. The zero approaches the origin as $n \to \infty$. We have sought, without success, to find a simple formula for x_n^*. We do not understand its origin or possible significance. Such behaviour also occurs in the

Table 2. Estimates of the zero point x_n^* and the physical critical index α_n for Ising model with external magnetic field. Estimates of the zero point x_n^{*2} and singularity amplitudes A_n, defined by (31), for the Heisenberg antiferromagnet with a staggered parallel magnetic field. Note the very high precision obtained for x_n^* for larger values of n.

	Ising model with an external magnetic field		Heisenberg antiferromagnet with a staggered parallel magnetic field	
n	x_n^*	α_n	x_n^{*2}	A_n
3		2.8(2)		0.070(3)
4	−0.1429(1)	4.3(5)	−0.44(5)	−0.089(6)
5	−0.070086(2)	5.9(9)	−0.195(10)	0.15(3)
6	−0.037303252(4)	7.9(8)	−0.0978(10)	−0.25(10)
7	−0.021347065(2)	9.2(10)	−0.05370(3)	0.4(2)
8	−0.0129118372(5)	11.1(8)	−0.031257(3)	
9	−0.0081442518(6)	13(2)	−0.0189613(10)	
10	−0.00530545634(4)	15(3)	−0.0118489(2)	
11	−0.0035446108572(5)	17(4)	−0.00756553(5)	

low-temperature series for the Euclidean Ising model but, to our knowledge, has not previously been remarked upon.

In order to locate the physical critical point x_c, we must firstly remove the above zero point. This can be done by dividing the original series by $x_n^* - x$ or by adding a constant to the original series, although neither procedure is entirely satisfactory. The resulting series show the physical singularity at x_c but with poor precision. Assuming the previous value $x_c = 0.579\,17(14)$ we obtain estimates of the exponent α_n which are also in table 2. These values have large uncertainty but are consistent with the scaling theory.

3.2. *Spin-$\frac{1}{2}$ Heisenberg antiferromagnet with external staggered parallel magnetic field*

The system can be described by the following Hamiltonian:

$$H = \sum_{\langle ij\rangle} S_i^z S_j^z + x \sum_{\langle ij\rangle} (S_i^x S_j^x + S_i^y S_j^y) + y\left(\sum_{i\in A} S_i^z - \sum_{j\in B} S_j^z\right) \qquad (27)$$

where the lattice has been divided into two sublattices A and B, and the limit $x = 1$ corresponds to the the isotropic Heisenberg model with staggered magnetic field. We have carried out the expansion of the ground-state energy E_0 up to order $(14, 11)$. The resulting series for the ground-state energy $E_0 = \sum E_{m,n} x^m y^n$ are listed in table 3. The calculations involve a list of 11 131 linked clusters of up to 14 sites, which were obtained previously (Zheng *et al* 1991).

The series can be analysed in a similar way as the series for the Ising model in subsection 3.1 above.

3.2.1. x grouping. We write

$$E_0 = \sum_m e_m(y) x^m \qquad (28)$$

with the $e_m(y)$ available as power series through e_{14} from the horizontal sequences in table 3. As before, we can find the exact expressions for $e_m(y)$ up to order $m = 6$

Table 3. Series coefficients for the ground-state energy per site E_0 of the Heisenberg antiferromagnet with an external staggered parallel magnetic field. Coefficients of $x^m y^n$ are listed.

m	$E_{m,0}$	$E_{m,1}$	$E_{m,2}$	$E_{m,3}$
0	−5.000000000000E − 1	−5.000000000000E − 1	0.000000000000E + 0	0.000000000000E + 0
2	−1.666666666667E − 1	1.111111111111E − 1	−7.407407407407E − 2	4.938271604938E − 2
4	9.259259259259E − 4	1.777777777778E − 2	−5.434567901235E − 2	1.006096021948E − 1
6	−1.581569664903E − 3	9.471293496823E − 3	−3.993589592823E − 2	1.221256691567E − 1
8	−8.252128462349E − 4	7.442915293815E − 3	−3.873953959277E − 2	1.511432514049E − 1
10	−3.118506492685E − 4	4.376910244841E − 3	−3.184889308437E − 2	1.630071345720E − 1
12	−2.419420797199E − 4	3.605706354343E − 3	−3.013798211966E − 2	1.821975709413E − 1
14	−1.511226784769E − 4	2.801005151458E − 3	−2.791500606737E − 2	1.980790896550E − 1

m	$E_{m,4}$	$E_{m,5}$	$E_{m,6}$	$E_{m,7}$
0	0.000000000000E + 0	0.000000000000E + 0	0.000000000000E + 0	0.000000000000E + 0
2	−3.292181069959E − 2	2.194787379973E − 2	−1.463191586648E − 2	9.754610577656E − 3
4	−1.485946776406E − 1	1.926526053955E − 1	−2.296466486613E − 1	2.584289990591E − 1
6	−2.938111701878E − 1	5.955074560284E − 1	−1.065752583745E + 0	1.738649381634E + 0
8	−4.799022350618E − 1	1.296996323312E + 0	−3.082499263371E + 0	6.607363039544E + 0
10	−6.607377784981E − 1	2.252869974451E + 0	−6.703566777064E + 0	1.785890236023E + 1
12	−8.797646937007E − 1	3.580396831391E + 0	−1.270851651862E + 1	4.030082558483E + 1
14	−1.115886548801E + 0	5.283429037504E + 0	−2.177572793248E + 1	8.003194275760E + 1

m	$E_{m,8}$	$E_{m,9}$	$E_{m,10}$	$E_{m,11}$
0	0.000000000000E + 0	0.000000000000E + 0	0.000000000000E + 0	0.000000000000E + 0
2	−6.503073718437E − 3	4.335382478958E − 3	−2.890254985972E − 3	1.926836657315E − 3
4	−2.791788035759E − 1	2.928281785578E − 1	−3.006406544334E − 1	3.039361522594E − 1
6	−2.643651773960E + 0	3.807048535328E + 0	−5.254484192346E + 0	7.013962178696E + 0
8	−1.302903809482E + 1	2.400580763108E + 1	−4.184037559705E + 1	6.966786618865E + 1
10	−4.342579996244E + 1	9.784899488089E + 1	−2.068084143229E + 2	4.140980229076E + 2
12	−1.162693987546E + 2	3.095702874107E + 2	−7.695530143378E + 2	1.803346351981E + 3
14	−2.670179747182E + 2	8.200682111741E + 2	−2.344661960983E + 3	6.299179304941E + 3

as follows:

$$e_0(y) = -(y+1)/2 \tag{29a}$$

$$e_2(y) = -\frac{3y+5}{2y+3} \tag{29b}$$

$$e_4(y) = \frac{1+23\,y+20\,y^2}{8(y+1)(2\,y+3)^3(4\,y+5)} \tag{29c}$$

$$\begin{aligned} e_6(y) = {} & -[32\,283 + 145\,336\,y + 419\,348\,y^2 + 1069\,752\,y^3 + 1926\,453\,y^4 \\ & + 2114\,694\,y^5 + 1340\,496\,y^6 + 451\,008\,y^7 + 62\,208\,y^8]/[48(y+2)(y+1)^3 \\ & \times (2\,y+3)^5(4\,y+5)^2(6\,y+7)(6\,y+5)]. \end{aligned} \tag{29d}$$

3.2.2. y grouping. We write

$$E_0 = \sum_n \mathcal{E}_n(x) y^n \tag{30}$$

where the $\mathcal{E}_n(x)$ are available as power series through x^{14} from the columns in table 3. Note that only even powers of x occur. The series $\mathcal{E}_0(x)$, $\mathcal{E}_1(x)$, $\mathcal{E}_2(x)$ are respectively the series for the ground-state energy, staggered magnetization and staggered parallel susceptibility in zero field, and agree with our previous results (Zheng *et al* 1991).

The critical point here is $x = 1$. Spin-wave theory (Zheng *et al* 1991) predicts the asymptotic behaviour

$$\mathcal{E}_n(x) \sim A_n(1-x^2)^{3/2-n} \qquad n \geqslant 2. \tag{31}$$

Analysis of these series by standard Dlog Padé approximants again shows a zero on the negative real x^2 axis (i.e. imaginary x) so that

$$\mathcal{E}_n(x) = (x_n^{*2} - x^2)\bar{\mathcal{E}}_n(x). \tag{32}$$

We give estimates of x_n^{*2} in table 2. The Dlog Padé approximants also identify the physical critical point and exponent, consistent with the spin-wave predictions, but with poor accuracy. Assuming these values we obtain estimates of the amplitudes A_n by forming the series for $(1-x^2)^{n-3/2}\mathcal{E}_n(x)$, transforming to the variable $\delta = 1-(1-x^2)^{1/2}$, and integrating the resulting Dlog Padé approximants. The estimates of A_n are also shown in table 2 (for $n \geqslant 7$, the series are too short to get reliable estimates).

3.3. Spin-$\frac{1}{2}$ Heisenberg antiferromagnet with external perpendicular magnetic field

This system is described by the following Hamiltonian:

$$H = \sum_{\langle ij \rangle} S_i^z S_j^z + x\sum_{\langle ij \rangle}(S_i^x S_j^x + S_i^y S_j^y) + y\sum_i S_i^x. \tag{33}$$

The limit $x = 1$ corresponds to the isotropic Heisenberg antiferromagnet with uniform magnetic field. In order to calculate the staggered magnetization M and staggered parallel susceptibility χ, we need to include an extra term

$$z\left(\sum_{i\in A} S_i^z - \sum_{j\in B} S_j^z\right) \tag{34}$$

in the above Hamiltonian.

Each of these quantities is expressed as a double power series in the variables x and y:

$$E_0 = \sum_{m,n=0} E_{m,n}x^m y^n \quad M = \sum_{m,n=0} M_{m,n}x^i y^j \quad \chi = \sum_{m,n=0} \chi_{m,n}x^m y^n \tag{35}$$

with the coefficients listed in table 4 through order 12 in y and through order 10–6 in x, depending on the order of y. Only even powers of y occur. The calculations involve the same linked-cluster data as used for the Ising model in subsection 3.1.

Table 4. Series coefficients for the ground-state energy per site E_0, staggered magnetization M, and staggered parallel susceptibility χ of the Heisenberg antiferromagnet with an external perpendicular magnetic field. Coefficients of $x^m y^{2n}$ are listed.

m	$E_{m,0}$	$E_{m,2}$	$E_{m,4}$	$E_{m,6}$	$E_{m,8}$	$E_{m,10}$	$E_{m,12}$
0	−5.000000000000E−1	−1.250000000000E−1	−2.604166666667E−3	−1.627604166667E−4	−5.114520037616E−5	−5.447831173493E−6	−2.633813829587E−6
1	0.000000000000E+0	1.666666666667E−1	7.812500000000E−3	1.509150752315E−3	3.338073604882E−4	9.978668513838E−5	2.507725096592E−5
2	−1.666666666667E−1	−1.770833333333E−1	−1.952039930556E−2	−5.091223445939E−3	−1.782273061596E−3	−5.668371892675E−4	−2.226080523312E−4
3	0.000000000000E+0	1.898148148148E−1	3.440679655350E−2	1.450564927356E−2	6.114337815663E−3	2.718367047858E−3	1.193310049978E−3
4	9.259259259259E−4	−1.917611239712E−1	−5.674982515583E−2	−3.221153197922E−2	−1.845058511270E−2	−9.908818775843E−3	−5.189127562187E−3
5	0.000000000000E+0	1.965794618362E−1	8.241384294860E−2	6.575710408563E−2	4.713958950604E−2	3.098326075623E−2	1.898943071618E−2
6	−1.581569664903E−3	−1.979340045037E−1	−1.162081313516E−1	−1.206513565578E−1	−1.084900898943E−1	−8.531757304614E−2	−6.122464754459E−2
7	0.000000000000E+0	2.014771059643E−1	1.544132116317E−1	2.073587033484E−1	2.281404047833E−1	2.136107300484E−1	
8	−8.252128462349E−4	−2.026578233458E−1	−1.996198231384E−1	−3.356520743631E−1	−4.482850607972E−1		
9	0.000000000000E+0	2.046074907859E−1	2.498565479032E−1	5.206316819720E−1			
10	−3.118506492685E−4	−2.055138486607E−1					

m	$M_{m,0}$	$M_{m,2}$	$M_{m,4}$	$M_{m,6}$	$M_{m,8}$	$M_{m,10}$	$M_{m,12}$
0	5.000000000000E−1	−6.250000000000E−2	−1.085069444444E−2	−2.292209201389E−3	−7.901792173032E−4	−2.198079056210E−4	−8.500195667112E−5
1	0.000000000000E+0	1.944444444444E−1	5.577256944444E−2	2.120424623843E−2	8.042577971156E−3	3.304592882101E−3	1.283906078619E−3
2	−1.111111111111E−1	−3.515625000000E−1	−1.873104745370E−1	−9.556587912477E−2	−4.922231540087E−2	−2.363877938519E−2	−1.155937734747E−2
3	0.000000000000E+0	5.577546296296E−1	4.509905285494E−1	3.269123502997E−1	2.078886428507E−1	1.246404167359E−1	7.064350932148E−2
4	−1.777777777778E−2	−7.524038708848E−1	−9.393134918925E−1	−8.914846281207E−1	−7.195486587872E−1	−5.152194980087E−1	−3.415279131472E−1
5	0.000000000000E+0	9.814607252124E−1	1.704622602543E+0	2.132678921263E+0	2.111460217567E+0	1.801538338863E+0	1.382343619444E+0
6	−9.471293496823E−3	−1.197304120927E+0	−2.875312008925E+0	−4.555172846613E+0	−5.495752441134E+0	−5.519147237135E+0	−4.879398295741E+0
7	0.000000000000E+0	1.444128162417E+0	4.513708148783E+0	8.959360671918E+0	1.297204712514E+1	1.522957418573E+1	
8	−7.442915293815E−3	−1.678066001724E+0	−6.755979144525E+0	−1.644348559772E+1	−2.831428309100E+1		
9	0.000000000000E+0	1.931941596993E+0	9.683391145493E+0	2.856987464341E+1			
10	−4.376910244841E−3	−2.177511665422E+0					

m	$\chi_{m,0}$	$\chi_{m,2}$	$\chi_{m,4}$	$\chi_{m,6}$	$\chi_{m,8}$	$\chi_{m,10}$	$\chi_{m,12}$
0	0.000000000000E+0	6.250000000000E−2	3.790509259259E−2	1.694742838542E−2	8.689894028652E−3	3.784368179977E−3	1.823280115110E−3
1	0.000000000000E+0	−3.425925925926E−1	−2.749204282407E−1	−1.873964919102E−1	−1.098907025533E−1	−6.237756403287E−2	−3.265108314236E−2
2	1.481481481481E−1	9.341724537037E−1	1.194185962818E+0	1.035323275846E+0	7.774303309472E−1	5.137212508745E−1	3.219827672035E−1
3	0.000000000000E+0	−2.047635030864E+0	−3.610283168171E+0	−4.181915248547E+0	−3.797638124116E+0	−3.022649032705E+0	−2.178772318343E+0
4	1.086913580247E−1	3.542967465242E+0	9.099571651374E+0	1.331847293491E+1	1.486971016386E+1	1.390420417788E+1	1.155187005604E+1
5	0.000000000000E+0	−5.732439735457E+0	−1.955684381601E+1	−3.647391253217E+1	−4.895221886920E+1	−5.362981002811E+1	−5.098845342144E+1
6	7.987179185646E−2	8.314889564378E+0	3.823478696672E+1	8.818028084421E+1	1.415360176471E+2	1.800845689230E+2	1.951087450144E+2
7	0.000000000000E+0	−1.173063336362E+1	−6.853930816031E+1	−1.941068762844E+2	−3.683252620670E+2	−5.412138340913E+2	
8	7.747907918554E−2	1.556572464104E+1	1.156292003543E+2	3.952020479146E+2	8.800409893333E+2		
9	0.000000000000E+0	−2.026268687267E+1	−1.848417959583E+2	−7.555037861516E+2			
10	6.369778616875E−2	2.543016317370E+1					

In this case we have not considered an x grouping of the series. The columns in table 4 give series in x for the quantities

$$\mathcal{E}_n(x) = \sum_m E_{m,n} x^m$$
$$\mathcal{M}_n(x) = \sum_m M_{m,n} x^m \qquad (36)$$
$$\overline{\chi}_n(x) = \sum_m \chi_{m,n} x^m$$

which represent field-derivatives of E_0, M and χ. The series for $\mathcal{E}_0(x)$, $\mathcal{E}_1(x)$, $\mathcal{M}_0(x)$ and $\overline{\chi}_0(x)$ agree with our previous results (Zheng *et al* 1991).

Analysis of the series for $\mathcal{E}_n(x)$, $\mathcal{M}_n(x)$ and $\overline{\chi}_n$ by Dlog Padé approximants again show a zero near the origin, but on the positive real x axis. The zero occurs in the series with $n = 2, 6, 10$ but not for $n = 4, 8, 12$. We do not understand the significance of this. The locations of the zero points are shown in table 5.

Table 5. The zero point x_n^* and the critical index α_n, estimated by analysing the series $\mathcal{E}_n$, $\mathcal{M}_n$ and $\overline{\chi}_n$ for the Heisenberg antiferromagnet with an external perpendicular magnetic field.

	$\mathcal{E}_2$	$\mathcal{E}_4$	$\mathcal{E}_6$	$\mathcal{E}_8$	$\mathcal{E}_{10}$
x_n^*			0.1732(4)		0.0806(1)
α_n	1.1(1)	3.3(4)	6.0(3)	10(3)	
	$\mathcal{M}_2$	$\mathcal{M}_4$	$\mathcal{M}_6$	$\mathcal{M}_8$	$\mathcal{M}_{10}$
x_n^*	0.68(3)		0.249(2)		0.158(3)
α_n	2.2(2)	4.6(4)	7.0(4)	10.5(15)	
	$\overline{\chi}_2$	$\overline{\chi}_4$	$\overline{\chi}_6$	$\overline{\chi}_8$	$\overline{\chi}_{10}$
x_n^*	0.374(2)		0.235(3)		0.17(2)
α_n	3.3(4)	6.0(4)	8.5(15)	11.7(7)	

In this case we expect physical critical points at both $x = -1$ and $x = 1$. At $x = -1$, spin-wave theory (Zheng *et al* 1991) predicts that the functions diverge:

$$\mathcal{E}_n(x),\ \ \mathcal{M}_n(x),\ \ \overline{\chi}_n(x) \sim (1+x)^{-\alpha_n} \qquad n \neq 0 \qquad (37)$$

but estimates of the exponent α_n are not known except for $\mathcal{E}_1(x)$, for which $\alpha_1 = 1$.

The Dlog Padé approximants show the singularity at $x = -1$ but with low precision. Assuming this value estimates for the exponents α_n can be obtained, and are also shown in table 5. These appear to increase linearly with n, suggesting a scaling relation with a gap exponent, as in subsection 3.1.

Near the other critical point $x = 1$ the functions are not expected to diverge. The series are difficult to analyse at this point. Using the method of Zheng *et al* (1991) we can obtain the following estimate:

$$E_0(1, y) = -0.6693(1) - 0.0659(10)y^2 - 0.0103(4)y^4 + 0.000\,45(9)y^6 + \mathrm{O}(y^8). \qquad (38)$$

4. Summary and discussion

We have developed a technique for deriving two-parameter series expansions for the ground-state energy and other ground-state properties of quantum spin systems involving two perturbing terms. This is an extension of our previous work with one parameter linked-cluster expansions.

The technique should be applicable to a number of interesting and incompletely understood systems, notably antiferromagnets with further-neighbour interactions. We are currently investigating such models.

As somewhat simpler applications of the method we have obtained two-parameter series for three models on the square lattice:

(i) the quantum Ising model with an external magnetic field,

(ii) the $S = \frac{1}{2}$ Heisenberg antiferromagnet (XXZ model) with an external staggered parallel magnetic field, and

(iii) the $S = \frac{1}{2}$ Heisenberg antiferromagnet with an external perpendicular magnetic field.

The series represent substantial new results for these models.

Analysis of the series has revealed, in most cases, a zero point near the origin, with the location and exponent (= 1) obtainable to very high accuracy. We do not understand the origin and significance of this. When the zero point is removed appropriately, the resulting series show behaviour consistent with scaling and spin-wave predictions, although the precision of estimates of critical parameters is only fair.

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