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Application of the connected-moments expansion to the $S = \frac{1}{2}$ Heisenberg antiferromagnet

K C Lee and C F Lo

Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong

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Abstract. In this paper we have applied the method of connected-moments expansion (CMX) to investigate the ground state of the spin-half ($S = \frac{1}{2}$) anisotropic Heisenberg antiferromagnet for linear chain, honeycomb, square, simple cubic and body-centred cubic lattices. For the case of isotropic exchange interaction, a detailed comparison has shown good agreement between the CMX results and those obtained by other methods. The convergence of the CMX is fairly rapid, and becomes better as the coordination number increases or the anisotropy parameter of exchange interaction decreases. Hence the CMX seems to be a practical tool for calculating the ground-state energy of a spin system since only the second- or third-order estimation will be needed in actual practice.

1. Introduction

In the past few decades the magnetic properties of an anisotropic quantum antiferromagnet have been extensively studied both theoretically and experimentally [1]. Here the anisotropy means either anisotropic exchange interactions or single-ionic-type anisotropy. Despite the apparent simplicity of the system, exact results are scarce. For instance, in the case of the isotropic spin-half ($S = \frac{1}{2}$) Heisenberg antiferromagnet, the exact ground state is known for the linear chain only, whereas beyond one dimension the exact nature of the ground state remains unknown [2, 3]. In recent years the interest in the quantum antiferromagnetic models has been further intensified by the discovery of the high-T_c superconductivity and Anderson's suggestion that there is a possible connection between the ground state of the high-T_c superconducting materials and the two-dimensional $S = \frac{1}{2}$ Heisenberg antiferromagnet [4, 5]. There have been many investigations, both analytical [6–11] and numerical [12, 13], on the ground-state properties of the $S = \frac{1}{2}$ system for various lattices. A pioneering analytical work known as the linear spin-wave (LSW) theory was given by Anderson and has proved to be quite successful in predicting the properties of the ground state (and even low-lying excited states) [6]. The LSW theory takes only the linear part under the Holstein–Primakoff transformation [14], and then a diagonalized Hamiltonian is obtained. In order to improve the result of LSW theory, one needs to resort to the perturbative series expansion [9, 10, 15]. However, since the spin-wave theory is an expansion in powers of $1/(zS)$, z being the coordination number, it is natural to raise doubts about the convergence of this expansion for low-spin and low-dimension (low-z) systems.

Recently, a new non-perturbative analytic method, the connected-moments expansion (CMX), for calculating ground-state energies of many-body systems, was developed by Cioslowski [16]. The method has been applied to various molecular Hamiltonians and is able to provide promising results [17–19]. The CMX was based on a theorem by Horn and Weinstein concerning the ground-state energy of a many-body system [20]. The theorem states that if $|\phi\rangle$ has non-zero overlap with the exact ground-state wave function of the system under consideraiton, then the function

$$F(t)=\frac{\langle\phi|\exp(-tH)H|\phi\rangle}{\langle\phi|\exp(-tH)|\phi\rangle}=\sum_{k=0}^{\infty}\frac{(-t)^k I_{k+1}}{k!} \tag{1}$$

converges to the exact ground-state energy E_0 at the limit $t\to\infty$. The coefficients I_k are connected moments of the Hamiltonian:

$$I_k=\langle\phi|H^k|\phi\rangle-\sum_{i=0}^{k-2}C_i^{k-1}I_{i+1}\langle\phi|H^{k-i-1}|\phi\rangle. \tag{2}$$

In practice, one is never able to generate the whole t-series for $F(t)$, and has to rely on some method of extracting E_0 from a finite number of terms of the t-expansion. It is clear that $F(t)$ is a monotonically decreasing function of t since the derivative of $F(t)$ with respect to t is equal to the negative of the expectation value of the operator $(H-\langle H\rangle)^2$. Moreover, both $F(t)$ and I_k scale linearly with N for any system of N independent particles, and thus both of them are size extensive. Owing to these properties, Cioslowski proposed that $F(t)$ can be written in the form

$$F(t)=E_0+\sum_{j=1}^{\infty}A_j\exp(-b_jt)\qquad b_j>0. \tag{3}$$

Next, by considering the following approximant to $F(t)$:

$$F(t)\simeq F_m(t)=E_0+\sum_{j=1}^{m}A_j\exp(-b_jt)\qquad b_j>0 \tag{4}$$

and by matching the power series of equation (1) and equation (4) at low order, one obtains

$$\sum_{j=1}^{m}A_jb_j^{k+1}=I_{k+2}\qquad k=0,1,2,\ldots,2m-1 \tag{5}$$

and

$$F_m(0)\equiv I_1=E_0+\sum_{j=1}^{m}A_j\Rightarrow E_0=I_1-\sum_{j=1}^{m}A_j=I_1+E_{\mathrm{corr}}^{(m)}. \tag{6}$$

Then the remaining work is to find an expression relating $E_{\mathrm{corr}}^{(m)}$ and the connected moments I_k. To achieve this, one introduces the function

$$f(t)=\sum_{k=0}^{\infty}I_{k+2}t^k \tag{7}$$

so that the coefficients A_j, b_j can be determined by matching the low-order terms in the power series of equation (7) with those of

$$f_m(t)=\sum_{j=1}^{m}\frac{A_jb_j}{1-b_jt}. \tag{8}$$

It is not difficult to show that the solution for $f_m(t)$ can be conveniently written as the quadratic form

$$f_m(t) = \boldsymbol{X}_m \mathbf{U}_m^{-1} \boldsymbol{X}_m^{\mathrm{T}} \tag{9}$$

where $\boldsymbol{X}_m$ is the row vector $(I_2, I_3, I_4, \ldots, I_{m+1})$, $\boldsymbol{X}_m^{\mathrm{T}}$ the transpose of $\boldsymbol{X}_m$ and $\mathbf{U}_m^{-1}$ the inverse of the matrix $\mathbf{U}_m$ defined by $(\mathbf{U}_m)_{ij} = I_{i+j} - tI_{i+j+1}$. Taking the limit $t \to \infty$ for the expression $tf_m(t)$, one finds the $E_{\mathrm{corr}}^{(m)}$:

$$E_{\mathrm{corr}}^{(m)} = \lim_{t\to\infty} tf_m(t) = -\boldsymbol{X}_m \mathbf{T}_m^{-1} \boldsymbol{X}_m^{\mathrm{T}} \tag{10}$$

where $\mathbf{T}_m^{-1}$ is the inverse of the matrix $\mathbf{T}_m$ defined by $(\mathbf{T}_m)_{ij} = I_{i+j+1}$. As a result, the CMX series for calculating the ground-state energy E_0 is given by [16, 21]

$$E_0 = I_1 - \lim_{n\to\infty} \boldsymbol{X}_n \mathbf{T}_n^{-1} \boldsymbol{X}_n^{\mathrm{T}}. \tag{11}$$

This CMX method has the property that the CMX series truncated at any order is always size extensive, and thus appears to be very attractive for many-body calculations. However, the applicability of the CMX method for ground-state energy is never granted *a priori*, and has to be carefully investigated for each Hamiltonian under consideration.

In the present work we adapt the CMX technique to the spin-lattice models and investigate its validity for this class of Hamiltonians. The specific lattice problem we have in mind is the $S = \frac{1}{2}$ Heisenberg antiferromagnet. This model has been extensively studied and thus should provide a good testing ground for the CMX method. We calculate the ground-state energy of the $S = \frac{1}{2}$ antiferromagnet for various lattices using the CMX series as well as investigating the convergence of these CMX results. So far as we know, the CMX method has not yet been applied to such systems despite the long history of attempts to improve on available methods for these lattice problems. The outline of this paper is as follows. In the next section we apply the CMX method to the $S = \frac{1}{2}$ Heisenberg antiferromagnet for various lattices such as linear chain, honeycomb, square, simple cubic and body-centred cubic lattices. Numerical results are then discussed in section 3.

2. Theory

The Hamiltonian of the $S = \frac{1}{2}$ Heisenberg antiferromagnet with anisotropic exchange interaction is given by

$$H = \frac{J}{2} \sum_{(i,j)} \{S_i^z S_j^z + R(S_i^x S_j^x + S_i^y S_j^y)\} = \frac{J}{2} \sum_{(i,j)} S_i^z S_j^z + \frac{JR}{4} \sum_{(i,j)} (S_i^+ S_j^- + S_i^- S_j^+) \tag{12}$$

where the spin-raising and lowering operators are defined by $S^{\pm} \equiv S^x \pm \mathrm{i}S^y$. Here J is a positive quantity representing the antiferromagnetic exchange interaction strength, R is the anisotropy parameter varying between zero and unity, and $\sum_{(i,j)}$ denotes the summation over all nearest-neighbour pairs. Anticipating antiferromagnetism we may rewrite the Hamiltonian by performing a rotation of the spin quantization axis at each site of one sublattice ('down' sublattice) into the direction of the local mean field. After the transformation the Hamiltonian becomes

$$H = H_0 + H_1 = -\frac{J}{2} \sum_{(i,j)} S_i^z S_j^z + \frac{JR}{4} \sum_{(i,j)} (S_i^+ S_j^+ + S_i^- S_j^-). \tag{13}$$

Table 1. Comparison of the first-order CMX results with LSW theory.

Lattice	γ	$\tilde{\gamma} \equiv z/[2(z-1)]$
Linear chain	0.726	1.0
Honeycomb	—	0.75
Square	0.632	0.667
SC	0.582	0.6
BCC	0.584	0.571

In this new basis the Hamiltonian H_0 is just the Hamiltonian of the ferromagnetic Ising model and its ground state $|\phi_0\rangle$ is well known, i.e. the state with all spins 'up': $|\phi_0\rangle \equiv \prod_{i=1}^{N} |\uparrow\rangle_i$. It is, therefore, natural to choose the state $|\phi_0\rangle$ as our starting state of the CMX for the Hamiltonian H. In fact, we believe that when R is small, the state $|\phi_0\rangle$ should be fairly close to the exact ground state. Once the starting state is fixed, it is straightforward, though tedious, to calculate various connected moments $I_k \equiv \langle\phi_0|H^k|\phi_0\rangle_c$ of H (either by hand or by computer), which in turn enable us to evaluate the ground-state energy using the CMX series. Since the calculations are quite lengthy, the details are not discussed here, and numerical results are presented in the next section. In the following we shall, however, discuss in more detail the first few terms of the CMX for the case of isotropic exchange interaction and compare the results with the LSW theory.

The first three connected moments of H for the isotropic case are given by

$$I_1 = -\tfrac{1}{8}JzN \tag{14}$$

$$I_2 = \tfrac{1}{8}J^2zN \tag{15}$$

$$I_3 = \tfrac{1}{8}J^3z(z-1)N. \tag{16}$$

Consequently, the zeroth- and first-order estimations of the ground-state energy of H are:

$$E_0^{(0)} = I_1 = -\tfrac{1}{8}JzN \tag{17}$$

$$E_0^{(1)} = I_1 - \frac{I_2^2}{I_3} = -\tfrac{1}{8}JzN\left\{\frac{1}{1-z^{-1}}\right\} = -\tfrac{1}{8}JzN\left\{1 + \frac{1}{z} + \left[\frac{1}{z}\right]^2 + \cdots\right\}. \tag{18}$$

According to Anderson's LSW theory, a rough estimation of the ground-state energy is given by [6]

$$E_0^{\mathrm{LSW}} \simeq -\tfrac{1}{8}JzN\left\{1 + \frac{1}{z}\right\}. \tag{19}$$

Thus comparing equation (18) with equation (19) suggests that within the first-order estimation the CMX is able to recover the LSW results, at least for large z. More precise LSW results are given in the following form:

$$E_0^{\mathrm{LSW}} = -\tfrac{1}{8}JzN\left\{1 + \frac{2\gamma}{z}\right\}. \tag{20}$$

The value corresponding to γ in our first-order CMX estimation is $\tilde{\gamma} \equiv z/[2(z-1)]$. For a further comparison we tabulate the values of γ and $\tilde{\gamma}$ for various z in table 1. It is clear that γ and $\tilde{\gamma}$ are in fairly good agreement, at least for large z.

3. Numerical results

We have calculated the connected moments I_k of the $S = \frac{1}{2}$ anisotropic Heisenberg antiferromagnet up to $k = 11$ for various lattices, and they are listed in the appendix. In terms of these connected moments we can derive the CMX of the ground-state energy per spin up to the fifth order. In tables 2–6 the numerical results for various lattices with different R are tabulated. From the numerical data it is observed that for small values of R the CMX shows a convergent pattern and limits can be reached for quite a low order of the expansion. This is actually not surprising because the Néel state is taken to be the starting state for the expansion, and it is supposed to be fairly close to the exact ground state when R is small.

Table 2. CMX results for the linear chain.

R	$E_0^{(0)}$	$E_0^{(1)}$	$E_0^{(2)}$	$E_0^{(3)}$	$E_0^{(4)}$	$E_0^{(5)}$
0.1	−0.25	−0.2525	−0.252 486	−0.252 493	−0.252 494	−0.252 494
0.2	−0.25	−0.26	−0.259 780	−0.259 857	−0.259 915	−0.259 898
0.3	−0.25	−0.2725	−0.271 416	−0.271 725	−0.271 175	−0.271 952
0.4	−0.25	−0.29	−0.286 697	−0.287 557	−0.287 468	−0.288 071
0.5	−0.25	−0.3125	−0.304 795	−0.306 765	−0.306 764	−0.307 464
0.6	−0.25	−0.34	−0.324 844	−0.328 801	−0.328 703	−0.329 509
0.7	−0.25	−0.3725	−0.346 031	−0.353 216	−0.352 659	−0.353 682
0.8	−0.25	−0.41	−0.367 647	−0.379 679	−0.378 071	−0.379 516
0.9	−0.25	−0.4525	−0.389 116	−0.407 971	−0.404 464	−0.406 639
1.0	−0.25	−0.5	−0.41	−0.437 965	−0.431 436	−0.434 784

Table 3. CMX results for the honeycomb lattice.

R	$E_0^{(0)}$	$E_0^{(1)}$	$E_0^{(2)}$	$E_0^{(3)}$	$E_0^{(4)}$	$E_0^{(5)}$
0.1	−0.375	−0.376 875	−0.376 871	−0.376 872	−0.376 872	−0.376 872
0.2	−0.375	−0.3825	−0.382 434	−0.382 453	−0.382 457	−0.382 457
0.3	−0.375	−0.391 875	−0.391 543	−0.391 629	−0.391 674	−0.391 662
0.4	−0.375	−0.405	−0.403 966	−0.404 215	−0.404 743	−0.404 341
0.5	−0.375	−0.421 875	−0.419 397	−0.419 970	−0.419 658	−0.420 288
0.6	−0.375	−0.4425	−0.437 479	−0.438 632	−0.438 508	−0.439 222
0.7	−0.375	−0.466 875	−0.457 817	−0.459 931	−0.459 898	−0.460 806
0.8	−0.375	−0.495	−0.480 000	−0.483 611	−0.483 611	−0.484 725
0.9	−0.375	−0.526 88	−0.503 620	−0.509 443	−0.509 365	−0.510 709
1.0	−0.375	−0.5625	−0.528 285	−0.537 228	−0.536 879	−0.538 521

For larger values of R the CMX appears to converge more slowly due to the quantum fluctuations. Since the quantum fluctuations will be more dominant in low dimensions, we may expect better CMX results for higher dimensions. In fact, this can be easily seen by inspecting the numerical data of the isotropic case for various lattices. In table 7 the ground-state energies for the one-, two- and three-dimensional lattices obtained by various methods are listed. It can be seen that our CMX results agree with them fairly well, especially in the three-dimensional case, and that even the second-order CMX is sufficient to give a reasonable estimate of the ground-state energy. This suggests that the first few orders of the CMX have already recovered a large portion of the ground-state energy.

Table 4. CMX results for the square lattice.

R	$E_0^{(0)}$	$E_0^{(1)}$	$E_0^{(2)}$	$E_0^{(3)}$	$E_0^{(4)}$	$E_0^{(5)}$
0.1	−0.5	−0.501 667	−0.501 667	−0.501 667	−0.501 667	−0.501 667
0.2	−0.5	−0.506 667	−0.506 645	−0.506 664	−0.506 665	−0.506 665
0.3	−0.5	−0.515 000	−0.514 893	−0.514 977	−0.514 995	−0.514 994
0.4	−0.5	−0.526 667	−0.526 329	−0.526 567	−0.526 666	−0.526 650
0.5	−0.5	−0.541 667	−0.540 848	−0.541 368	−0.541 745	−0.541 635
0.6	−0.5	−0.560 000	−0.558 318	−0.559 283	−0.560 656	−0.559 956
0.7	−0.5	−0.581 667	−0.578 581	−0.580 194	−0.592 200	−0.581 635
0.8	−9.5	−0.606 667	−0.601 463	−0.603 969	−0.598 668	−0.606 726
0.9	−0.5	−0.635 000	−0.626 772	−0.630 466	−0.627 537	−0.635 352
1.0	−0.5	−0.666 667	−0.654 303	−0.659 536	−0.657 394	−0.667 808

Table 5. CMX results for the simple cubic lattice.

R	$E_0^{(0)}$	$E_0^{(1)}$	$E_0^{(2)}$	$E_0^{(3)}$	$E_0^{(4)}$	$E_0^{(5)}$
0.1	−0.75	−0.7515	−0.751 499	−0.751 500	−0.751 500	−0.751 500
0.2	−0.75	−0.756	−0.755 991	−0.755 999	−0.755 999	−0.755 999
0.3	−0.75	−0.7635	−0.763 454	−0.763 493	−0.763 497	−0.763 497
0.4	−0.75	−0.774	−0.773 854	−0.773 973	−0.773 995	−0.773 993
0.5	−0.75	−0.7875	−0.787 145	−0.787 421	−0.787 502	−0.787 490
0.6	−0.75	−0.804	−0.803 266	−0.803 806	−0.804 045	−0.803 995
0.7	−0.75	−0.8235	−0.822 147	−0.823 091	−0.823 699	−0.823 520
0.8	−0.75	−0.846	−0.843 704	−0.845 226	−0.846 677	−0.846 081
0.9	−0.75	−0.8715	−0.867 846	−0.870 156	−0.873 705	−0.871 700
1.0	−0.75	−0.9	−0.894 470	−0.897 816	−0.909 082	−0.900 393

Table 6. CMX results for the body-centred cubic lattice.

R	$E_0^{(0)}$	$E_0^{(1)}$	$E_0^{(2)}$	$E_0^{(3)}$	$E_0^{(4)}$	$E_0^{(5)}$
0.1	−1.0	−1.001 429	−1.001 429	−1.001 429	−1.001 429	−1.001 429
0.2	−1.0	−1.005 714	−1.005 713	−1.005 722	−1.005 722	−1.005 722
0.3	−1.0	−1.012 857	−1.012 853	−1.012 897	−1.012 898	−1.012 898
0.4	−1.0	−1.022 857	−1.022 843	−1.022 981	−1.022 990	−1.022 989
0.5	−1.0	−1.035 714	−1.035 679	−1.036 017	−1.036 049	−1.036 047
0.6	−1.0	−1.051 429	−1.051 356	−1.052 055	−1.052 155	−1.052 147
0.7	−1.0	−1.07	−1.069 866	−1.071 156	−1.071 423	−1.071 396
0.8	−1.0	−1.091 429	−1.091 200	−1.093 393	−1.094 031	−1.093 950
0.9	−1.0	−1.115 714	−1.115 348	−1.118 847	−1.120 258	−1.120 026
1.0	−1.0	−1.142 857	−1.142 299	−1.144 606	−1.150 562	−1.149 919

In summary, we have applied the method of connected-moments expansion to investigate the ground state of the $S = \frac{1}{2}$ Heisenberg antiferromagnet. The connected-moments expansion of the ground-state energy up to the fifth order has been performed for linear chain, honeycomb, square, simple cubic and body-centred cubic lattices. For the case of isotropic exchange interaction, a detailed comparison has shown good agreement between the CMX results and those obtained by other methods; in fact, the first-order CMX estimation may be compared with the linear spin-wave theory of Anderson. The convergence of the CMX is fairly rapid, and becomes better as the coordination number increases or the anisotropy parameter of exchange interaction decreases. Besides, since our choice of the Néel state as the starting state is dictated primarily by our desire to use a calculationally

Table 7. Ground-state energy per spin from other methods for the isotropic Heisenberg antiferromagnet.

Method	E_0/J
Linear chain	
Exact result [2, 3]	−0.443 15
CMX result	−0.434 784
Honeycomb	
Bartkowski (variational) [8]	−0.5295
Kim and Hong (projection technique) [22]	−0.5409
CMX result	−0.538 521
Square lattice	
Anderson (spin waves) [6]	−0.658
Bullock (perturbational) [23]	−0.666
Singh (series expansion) [25]	−0.6696
Bartkowski (variational) [8]	−0.659
Kim and Hong (projection technique) [22]	−0.6674
Trivedi and Ceperley (GFMC) [13]	−0.6692
Liu and Manousakis (VMC) [26]	−0.6637
Tang and Hirsch (exact diagonalization) [27]	−0.672
CMX result	−0.667 808
Simple cubic	
Anderson (spin waves) [6]	−0.896
Bullock (perturbational) [23]	−0.900
Bartkowski (variational) [8]	−0.899
Kim and Hong (projection technique) [22]	−0.9009
CMX result	−0.900 393
Body centred cubic	
Kubo (spin waves) [24]	−1.151
Parrinello and Arai (perturbational) [10]	−1.1496
Bartkowski (variational) [8]	−1.153
Kim and Hong (projection technique) [22]	−1.148
CMX result	−1.149 919

manageable starting state and may not be a good one at all, especially for the isotropic case, one may improve the convergence of the CMX by using a better starting state, e.g. the Gutzwiller-type trial wave function. Furthermore, according to our calculations, the first few orders of the CMX have already recovered a large portion of the ground-state energy. Hence the CMX seems to be a practical tool for calculating ground-state energy of a spin system since only the second- or third-order estimation will be needed in actual practice.

Appendix

A1. Linear chain

$$I_1 = -\tfrac{1}{4}JN$$

$$I_2 = \tfrac{1}{4}R^2J^2N$$

$$I_3 = \tfrac{1}{4}R^2J^3N$$

$$I_4 = -\tfrac{1}{8}(3R^4 - 2R^2)J^4N$$
$$I_5 = -\tfrac{1}{4}(7R^4 - R^2)J^5N$$
$$I_6 = \tfrac{1}{8}(20R^6 - 43R^4 + 2R^2)J^6N$$
$$I_7 = \tfrac{1}{8}(213R^6 - 110R^4 + 2R^2)J^7N$$
$$I_8 = -\tfrac{1}{16}(595R^8 - 2684R^6 + 510R^4 - 4R^2)J^8N$$
$$I_9 = -\tfrac{1}{4}(2831R^8 - 3279R^6 + 279R^4 - R^2)J^9N$$
$$I_{10} = \tfrac{1}{8}(7812R^{10} - 60\,723R^8 + 27\,584R^6 - 1179R^4 + 2R^2)J^{10}N$$
$$I_{11} = \tfrac{1}{8}(233\,141R^{10} - 486\,110R^8 + 105\,307R^6 - 2438R^4 + 2R^2)J^{11}N.$$

A2. Honeycomb

$$I_1 = -\tfrac{3}{8}JN$$
$$I_2 = \tfrac{3}{8}R^2J^2N$$
$$I_3 = \tfrac{3}{4}R^2J^3N$$
$$I_4 = -\tfrac{1}{16}(15R^4 - 24R^2)J^4N$$
$$I_5 = (3R^2 - 9R^4)J^5N$$
$$I_6 = \tfrac{1}{8}(93R^6 - 462R^4 + 48R^2)J^6N$$
$$I_7 = \tfrac{1}{8}(2019R^6 - 2484R^4 + 96R^2)J^7N$$
$$I_8 = -\tfrac{1}{32}(10\,707R^8 - 106\,656R^6 + 48\,432R^4 - 768R^2)J^8N$$
$$I_9 = -\tfrac{1}{2}(25\,731R^8 - 69\,249R^6 + 13\,887R^4 - 96R^2)J^9N$$
$$I_{10} = \tfrac{1}{32}(557\,919R^{10} - 9\,207\,228R^8 + 9\,965\,016R^6 - 979\,536R^4 + 3072R^2)J^{10}N$$
$$I_{11} = \tfrac{1}{16}(16\,648\,221R^{10} - 78\,284\,160R^8 + 40\,708\,890R^6 - 2\,101\,176R^4 + 3072R^2)J^{11}N.$$

A3. Square lattice

$$I_1 = -\tfrac{1}{2}JN$$
$$I_2 = \tfrac{1}{2}R^2J^2N$$
$$I_3 = \tfrac{3}{2}R^2J^3N$$
$$I_4 = -\tfrac{1}{4}(5R^4 - 18R^2)J^4N$$
$$I_5 = -\tfrac{1}{2}(41R^4 - 27R^2)J^5N$$
$$I_6 = \tfrac{1}{4}(64R^6 - 861R^4 + 162R^2)J^6N$$
$$I_7 = \tfrac{1}{4}(2499R^6 - 7390R^4 + 486R^2)J^7N$$
$$I_8 = -\tfrac{1}{8}(3671R^8 - 113\,684R^6 + 113\,250R^4 - 2916R^2)J^8N$$
$$I_9 = -\tfrac{1}{2}(66\,681R^8 - 492\,845R^6 + 202\,121R^4 - 2187R^2)J^9N$$
$$I_{10} = \tfrac{1}{8}(186\,561R^{10} - 10\,713\,882R^8 + 28\,940\,408R^6 - 5\,507\,562R^4 + 26\,244R^2)J^{10}N$$
$$I_{11} = \tfrac{1}{4}(7\,948\,116R^{10} - 157\,774\,710R^8 + 189\,874\,417R^6 - 18\,163\,750R^4 + 39\,366R^2)J^{11}N.$$

A4. Simple cubic

$$I_1 = -\tfrac{3}{4}JN$$
$$I_2 = \tfrac{3}{4}R^2J^2N$$
$$I_3 = \tfrac{15}{4}R^2J^3N$$
$$I_4 = -\tfrac{1}{8}(21R^4 - 150R^2)J^4N$$
$$I_5 = -\tfrac{1}{4}(297R^4 - 375R^2)J^5N$$
$$I_6 = \tfrac{1}{8}(516R^6 - 10\,773R^4 + 3750R^2)J^6N$$
$$I_7 = \tfrac{1}{8}(30\,963R^6 - 159\,738R^4 + 18\,750R^2)J^7N$$
$$I_8 = -\tfrac{1}{16}(70\,137R^8 - 2\,306\,820R^6 + 4\,226\,130R^4 - 187\,500R^2)J^8N$$
$$I_9 = -\tfrac{1}{4}(1\,666\,521R^8 - 16\,931\,289R^6 + 13\,005\,297R^4 - 234\,375R^2)J^9N$$
$$I_{10} = \tfrac{1}{8}(9\,494\,817R^{10} - 199\,479\,885R^8 + 855\,724\,416R^6 - 305\,026\,293R^4 + 2\,343\,750R^2)J^{10}N$$
$$I_{11} = \tfrac{1}{8}(1\,172\,463\,867R^{10} - 9\,429\,456\,642R^8 + 19\,481\,911\,317R^6 - 3\,457\,012\,338R^4 + 11\,718\,750R^2)J^{11}N.$$

A5. Body centred cubic

$$I_1 = -JN$$
$$I_2 = R^2J^2N$$
$$I_3 = 7R^2J^3N$$
$$I_4 = -\tfrac{1}{2}(3R^4 - 98R^2)J^4N$$
$$I_5 = (-103R^4 + 343R^2)J^5N$$
$$I_6 = \tfrac{1}{2}(128R^6 - 6571R^4 + 4802R^2)J^6N$$
$$I_7 = \tfrac{1}{2}(9747R^6 - 154\,994R^4 + 33\,614R^2)J^7N$$
$$I_8 = \tfrac{1}{4}(7511R^8 + 1\,150\,340R^6 - 6\,233\,550R^4 + 470\,596R^2)J^8N$$
$$I_9 = (-39\,203R^8 + 14\,076\,045R^6 - 28\,456\,359R^4 + 823\,543R^2)J^9N$$
$$I_{10} = \tfrac{1}{4}(706\,425R^{10} - 92\,107\,566R^8 + 2\,331\,013\,288R^6 - 1\,951\,383\,462R^4 + 23\,059\,204R^2)J^{10}N$$
$$I_{11} = \tfrac{1}{4}(788\,839\,519R^{10} - 10\,493\,722\,636R^8 + 84\,438\,667\,826R^6 - 32\,028\,742\,612R^4 + 161\,414\,428R^2)J^{11}N.$$

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