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Calculation of the ground-state energies of quantum antiferromagnets via the projection technique

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We calculate the ground-state energies of the quantum antiferromagnetic Heisenberg model for lattices such as the chain, honeycomb, square, simple cubic, and body-centered cubic via the projection technique using cumulants. The method has been introduced by Becker, Won, and Fulde and applied to the same model for a square lattice. According to our calculations, we conclude that the first-order approximation may be compared with the linear spin-wave theory of Anderson through the dynamical analogy, and the convergence of the projection method becomes better as the coordination number increases.

I. INTRODUCTION

The discovery of the high-T_c superconducting materials and Anderson's suggestion[1] for the ground state of the materials renewed interest in the quantum antiferromagnetic (QAFM) Heisenberg model on a plane. Anderson's suggestion implies that there is a possible connection between the ground state of the Cu-O plane of the high-T_c superconducting materials and the two-dimensional (2D) spin-$\frac{1}{2}$ antiferromagnet. In fact, the half-filled Hubbard Hamiltonian, which is studied as a model describing the high-T_c material, is transformed into the antiferromagnetic Heisenberg model[2] in the strong-coupling limit. Therefore, for the time being, the study of the ground state of the latter model is an attractive problem in condensed-matter physics.

Even before this remarkable discovery, the study of the ground state for the QAFM has been considered one of the typical problems of spin systems. The exact solution for a chain has been obtained by using Bethe ansatz,[3] and it has been provided as a standard in testing the results given by various approximate theories.

Calculating the ground-state energy of the QAFM Heisenberg model for various lattices may be an interesting subject in connection with studying the ground state of the model. There have been many analytical works,[4-9] and recently several numerical works[10,11] have been done. A pioneering analytical work known as the linear spin-wave (LSW) theory was given by Anderson[5] for a chain, square, and simple cubic lattice. The LSW theory takes only the linear part under the Holstein-Primakoff transformation,[12] and then a diagonalized Hamiltonian is obtained.

The ordinary process to improve the result of LSW theory is to perform a perturbative calculation. For the spin systems, however, Wick's theorem of quantum field theory is not directly applicable. To avoid this difficulty, Arai and Goodman[7] have developed a cumulant expansion method using Kubo's theorem on cumulants[13] and applied the method to the QAFM. Some years ago, Parinello and Arai[8] rearranged the perturbative expansion and extended it up to an infinite order. We use some of their results in comparing ours with others. Recently, a new analytic method which we use here has been given by Becker, Won, and Fulde.[9] They developed a new projection technique using cumulants in calculating the ground-state energy and applied to the 2D QAFM Heisenberg model on a square lattice. We briefly summarize the formalism here.

The system under consideration is composed of the unperturbed Hamiltonian H_0, whose eigenstates and eigenvalues are known, and the perturbed part H_1. Becker, Won, and Fulde expressed the ground-state energy E_0 as

$$E_0=\varepsilon_0+\langle\phi_0|H_1|\phi_0\rangle+\varphi(0)\ , \tag{1}$$

where ε_0 and $|\phi_0\rangle$ are the ground-state energy and wave function of H_0, respectively, and

$$\varphi(z)=\left\langle\phi_0\left|H_1^{\dagger}\frac{1}{z-(L_0+H_1)}H_1\right|\phi_0\right\rangle^{c}\ . \tag{2}$$

The superscript c in Eq. (2) means cumulant,[9,13] and L_0 is the Liouville operator defined as $L_0A\equiv H_0A-AH_0$, where A is an operator.

Introducing a Liouville space in which a cumulant is defined as an inner product and applying the projection technique[14] to Eq. (2), we can get the following expression for $\varphi(z)$:

$$\varphi(z)=\frac{(H_1|H_1)}{z-(H_1|LH_1)/(H_1|H_1)-M(z)/(H_1|H_1)}\ , \tag{3}$$

where $L=L_0+H_1$ and the inner product $(A|B)$ means the cumulant $\langle\phi_0|A^{\dagger}B|\phi_0\rangle^c$.

It is interesting to note that Eq. (3) is just the form of the Laplace transformed relaxation function in a dynamical theory developed by Mori.[15] For this reason the second and third terms of the denominator in Eq. (3) may be called the frequency and memory parts, respectively. These terminologies are meaningful only in explaining something related to dynamical concepts. Thus we will discuss some of our results on the analogy of dynamics in what follows. Furthermore, the memory function $M(z)$ can also be expressed in a form similar to Eq. (3) with a

new frequency and a new memory part. Thus the function $\varphi(z)$ is expressed in an infinite continued fraction[15] eventually.

In this work we apply this projection technique to various lattice such as chain, honeycomb, square,[9] simple cubic, and body-centered-cubic lattice, and calculate their ground-state energies. One of the objects of this paper is to express the ground-state energies in terms of the coordination number q and to appreciate the results. In our lowest-order (first-order) approximation, we can express our results in terms of q and give them a meaning in connection to LSW theory. In fact, our first-order results are pretty close to those of LSW theory. We will discuss the dynamical similarity between the two approximations in what follows. The other object is to see when the projection technique becomes more effective. According to our ground-state energy calculations for various lattices, we can insist that faster convergence of the approximation be obtained as the coordination number increases.

This paper is composed as follows. In Sec. II we present a brief formalism for the ground-state energy in terms of the cumulant for the QAFM Heisenberg model. In Sec. III we calculate the ground-state energies and give an appreciation for the results in comparison with LSW theory. We also perform second- and third-order approximations for the memory function $M(z)$ in this section. Finally, we present our ground-state energies for various lattices and some discussion in Sec. IV.

II. FORMALISM

Antiferromagnets may be described by the Heisenberg model with positive strength of exchange interaction. We restrict our interest to the isotropic system. Then the Hamiltonian is written as

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \ , \tag{4}$$

where the angular bracket means the nearest neighbor, $\mathbf{S}_j$ is the quantum spin operator at lattice site j, and J is a positive quantity representing the exchange interaction strength. The Hamiltonian (4) can be rewritten in terms of spin-raising and -lowering operators defined by $S_j^{\pm} \equiv S_j^x \pm i S_j^y$. Then we rewrite this again by performing a unitary transformation such that up spins in the Néel state are rotated π about S^x axis.[16] The unitarity under this transformation remains for lattices such as chain, honeycomb, square, simple cubic, and body-centered cubic. The eventual changes after the transformation are $S_j^{\pm} \rightarrow S_j^{\mp}$ and $S_j^z \rightarrow -S_j^z$, where j is a lattice site in a sublattice composed of up spins. Therefore, (4) is written as

$$\begin{aligned} H &= -J \sum_{\langle i,j \rangle} S_i^z S_j^z + \left[\frac{J}{2} \sum_{\langle i,j \rangle} S_i^+ S_j^+ + \frac{J}{2} \sum_{\langle i,j \rangle} S_i^- S_j^- \right] \\ &= H_0 + (H_I + H_I^{\dagger}) \\ &= H_0 + H_1 \ . \end{aligned} \tag{5}$$

In Eq. (5), H_0 is the Hamiltonian of the ferromagnetic Ising model whose ground state $|\phi_0\rangle$ is well known, i.e., all spins down. Thus it is chosen as an unperturbed Hamiltonian. The perturbed part H_1 is the sum of all operators which raise or lower a pair of nearest-neighbor spins.

For a system whose total number of lattice sites is N and the coordination number q, the total number of nearest-neighbor bonds is $\frac{1}{2}Nq$. Then the ground-state energy of the Hamiltonian H_0 is easily given by $\epsilon_0 = -J(-\frac{1}{2})^2(\frac{1}{2}Nq)$, and the total ground-state energy E_0 of Eq. (1) is given by $E_0 = -\frac{1}{8}JNq + \langle \phi_0 | H_1 | \phi_0 \rangle + \varphi(0)$. It is simple to show that $\langle \phi_0 | H_1 | \phi_0 \rangle = 0$, $(H_1 | H_1) = (H_I | H_I)$, and $(H_1 | L H_1) = (H_I | L H_I)$.

Since $\langle \phi_0 | H_I | \phi_0 \rangle = 0$,

$$\begin{aligned} (H_I | H_I) &= \langle \phi_0 | H_I^+ H_I | \phi_0 \rangle - \langle \phi_0 | H_I^{\dagger} | \phi_0 \rangle \langle \phi_0 | H_I | \phi_0 \rangle \\ &= \left[\frac{J}{2} \right]^2 \left\langle \phi_0 \left| \sum_{\langle i,j \rangle} S_i^- S_j^- \sum_{\langle l,m \rangle} S_l^+ S_m^+ \right| \phi_0 \right\rangle \ , \\ &= \left[\frac{J}{2} \right]^2 \left[\sum_{\langle i,j \rangle} \right] = \left[\frac{J}{2} \right]^2 \frac{1}{2} Nq \ . \end{aligned} \tag{6}$$

On the other hand, since $(H_I | H_I^{\dagger} H_I) = (H_I | H_I H_I) = 0$,

$$\begin{aligned} (H_I | L H_I) &= (H_I | L_0 H_I) = (H_I | (H_0 - \epsilon_0) H_I) \\ &= J(q-1)(H_I | H_I) \ . \end{aligned} \tag{7}$$

The quantity $J(q-1)$ represents the difference of eigenvalues of the operator H_0 for the states $H_I|\phi_0\rangle$ and $|\phi_0\rangle$.

Therefore, the ground-state energy E_0 is given by

$$E_0 = -\frac{J}{8} Nq + \varphi(0) \ , \tag{8}$$

where

$$\varphi(0) = \left[\frac{(J^2/8)Nq}{z - J(q-1) - M(z)/(H_I | H_I)} \right]_{z=0} \ . \tag{9}$$

The memory function $M(z)$ is represented by[9]

$$M(z) = \left[H_I^2 \left| \frac{1}{z - QLQ} H_I^2 \right. \right] \ , \tag{10}$$

where Q is a projection operator defined by $Q = 1 - |H_I)(H_I|/(H_I|H_I)$. Since J and N are not important variables, it is interesting to note that the ground-state energy is expressed only in terms of the coordination number q, except $M(0)$. Even though we are not able to express $M(0)$ in terms of q in this work, it may be possible, in principle, for the exact $M(0)$ to be expressed in terms of q, because q is the only variable to distinguish the lattices whose Néel states are bipartite. What we have to do to calculate the ground-state energy is to obtain the memory function $M(0)$ approximately.

III. APPROXIMATIONS

A. First-order approximation

As mentioned in Sec. I, the function $\varphi(z)$ is written in the form of an infinite continued fraction. It is a familiar method, truncating the infinite continued fraction at a

certain level to calculate it approximately. Our first-order approximation is setting $M(z)=0$, which is equivalent to truncating the continued fraction at a first level. Then we simply get the ground-state energy of first-order in terms of the coordination number q, i.e.,

$$E_0^{(1)}=-\frac{1}{8}JNq\left[\frac{1}{1-1/q}\right]$$
$$=-\frac{1}{8}JNq\left[1+\frac{1}{q}+\left[\frac{1}{q}\right]^2+\cdots\right], \quad (11)$$

where the second line is the expansion in powers of $1/q$.

As also indicated earlier, the function $\varphi(z)$ has the same form as the Laplace-transformed relaxation function of dynamical theory.[15] Therefore, setting $M(z)=0$ corresponds to a single-mode approximation if we look $\varphi(z)$ from the dynamical point of view. Since the LSW Hamiltonian is written as $H^{\mathrm{LSW}}=\sum_k \varepsilon(k)a_k^\dagger a_k+\text{const}$, the Laplace-transformed relaxation function of the magnon operator a_k has a single pole. Therefore, we have a valid reason to compare our first-order results with those of LSW theory.

According to Anderson,[4] a rough estimation of the ground-state energy is given by

$$E_0^{\mathrm{LSW}}\simeq-\frac{1}{8}JNq\left[1+\frac{1}{q}\right]. \quad (12)$$

Thus comparing (12) with (11) confirms that the two approximations may have a common physical ground, at least for large q. What we can suggest for the common ground right now is the dynamical similarity between the two theories. More precise values of LSW theory are given in the following form, i.e., $E_0^{\mathrm{LSW}}=-\frac{1}{8}JNq(1+2\gamma/q)$. The corresponding value to γ in our first-order approximation is $q/[2(q-1)]$. We show these values for various q in Table I for a further comparison.

B. Second-order approximation

The second-order approximation is to truncate the infinite continued fraction at a second level, which is equivalent to approximating $L=L_0$. Since $QL_0Q|H_I^2)=L_0|H_I^2)$, the memory function in the second-order approximations is given by

$$M^{(2)}(z)=\left[H_I^2\left|\frac{1}{z-L_0}H_I^2\right.\right]$$
$$=\left\langle\phi_0\left|H_I^{\dagger 2}\frac{1}{z-L_0}H_I^2\right|\phi_0\right\rangle-\frac{2(J/2)^4(Nq/2)^2}{z-2(q-1)J}. \quad (13)$$

TABLE I. Comparison of our first order with LSW theory.

Lattice (q)	γ	$q/[2(q-1)]$
Chain (2)	0.726	1.0
Honeycomb (3)		0.75
Square (4)	0.632	0.667
s.c. (6)	0.58	0.6
bcc	0.58	0.571

A similar technique used in obtaining (7) is applied to calculate the first term of Eq. (13). In this case we have to find the difference of eigenvalues of H_0 for the states $H_I^2|\phi_0\rangle$ and $|\phi_0\rangle$. The state $H_I^2|\phi_0\rangle$, however, is obtained by flipping four spins which make two pairs of nearest-neighbor bonds. Thus there are several classes of spin configurations depending on q, and each class has a different eigenvalue of L_0. The number of spin configurations in each class affects the first term of Eq. (13). We summarize each class of spin configuration and the number of configurations in the class for the state $H_I^2|\phi_0\rangle$ in Appendix A. We also show the results of $M^{(2)}(z)$ for various types of lattices in Appendix A.

C. Third-order approximation

In an ordinary way of approximating an infinite continued fraction, the third order is to truncate the continued fraction at a third level as we did just before. But in obtaining the second order we found that $H_I^2|\phi_0\rangle$ is composed of multiple eigenstates of the operator L_0. Therefore, the formalism for projecting onto a single vector in the Liouville space may not be appropriate in this case. Therefore, a more generalized projection technique[14,15] which projects onto multiple states must be adopted in the third-order calculation. Since Becker, Won, and Fulde[9] have already used this technique for the square lattice, we do not explain the method here in detail.

We let $|A_i)=L_0^i|H_I^2)$, $i=0,1,\ldots,n-1$, where n is the number of projected states. Then we write a memory function in a matrix form

$$\tilde{M}(z)=\frac{1}{z-[\tilde{\Omega}+\tilde{M}'(z)]\tilde{P}^{-1}}\tilde{P}, \quad (14)$$

where the tilde means matrix representation, $\tilde{P}_{ij}=(A_i|A_j)$, $\tilde{\Omega}_{ij}=(A_i|QLQA_j)$, and $\tilde{M}'_{ij}(z)$ is written as follows:

$$\tilde{M}'_{ij}(z)=\left[A_i'\left|LQ\hat{Q}\frac{1}{z-\hat{Q}QLQ\hat{Q}}\hat{Q}QLA_j\right.\right], \quad (15)$$

where $\hat{Q}=1-\sum_{i,j}|A_i)(A_j|/(A_i|A_j)$. Thus $M(z)$ of Eq. (10) is obtained by finding $\tilde{M}_{00}$.

The matrices $\tilde{P}$ and $\tilde{\Omega}$ are easily obtained. But $\tilde{M}'(z)$ cannot be obtained exactly. We use the same approximation technique in calculating $\tilde{M}'(z)$ as one used in the second-order approximation, i.e., setting $L=L_0$ in (15). We show, for example, the honeycomb lattice case in Appendix B.

IV. RESULTS AND DISCUSSIONS

We performed the calculations up to second order for all lattices treated in this paper, and for chain and honeycomb lattices the third order is also performed. For simple cubic and body-centered cubic, the second order gives already good results. Therefore, the third-order calculations for these lattices are not that meaningful. We list the ground-state energies obtained by the projection technique and other methods in Table II.

As discussed earlier, the first order is compared with

TABLE II. Ground-state energies of first, second, and third order, and other results.

Lattice (q)	$E_0^{(1)}$	$E_0^{(2)}$	$E_0^{(3)}$	Other results
Chain (2)	-0.5	-0.45	-0.4423	-0.443[b]
Honeycomb (3)	-0.5625	-0.5386	-0.5409	-0.5295[c]
Square (4)[a]	-0.6666	-0.6574	-0.6674	-0.6692[d]
sc (6)	-0.9	-0.8995		-0.9009[e]
bcc	-1.142	-1.148		-1.1496[e]

[a]Reference 9.
[b]Reference 3.
[c]Reference 6.
[d]Reference 11.
[e]Reference 8.

LSW theory from the dynamical point of view. As one can see in Table I, those two results become closer as the coordination number increases. It is also interesting to see in Table II that the second-order results are larger than the first-order results, which means the former is worse than the latter. The body-centered cubic, however, looks like an exceptional case. But it may not be understood as an exception according to the following explanation. That is, if we see the differences between the first and second orders in Table II, they decrease as the coordination number q increases, and eventually the second becomes smaller at $q=8$. Therefore, we conclude that the approximation technique used by Becker, Won, and Fulde and the present authors is more effective for a lattice having large q.

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APPENDIX A: SPIN CONFIGURATIONS OF $H_I^2|\phi_0\rangle$ AND $M^{(2)}(z)$

1. Chain

There are two classes of spin configurations of $H_I^2|\phi_0\rangle$ which give different eigenvalues of L_0. We show them in Fig. 1, and call them $|\omega_1\rangle$ and $|\omega_2\rangle$. The eigenvalue equations are written as $L_0|\omega_1\rangle=J|\omega_1\rangle$ and $L_0|\omega_2\rangle=2J|\omega_2\rangle$. The numbers of configurations are $2N$ and $N(N-5)$ for $|\omega_1\rangle$ and $|\omega_2\rangle$ classes, respectively.

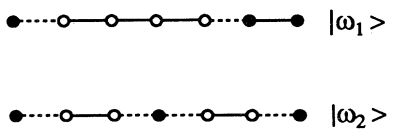

FIG. 1. Typical spin configurations of the eigenstates of L_0 in a chain. Black dots mean spin down and white does two pairs of flipped nearest-neighbor up spins.

Therefore,

$$M^{(2)}(z)=(J/2)^4N\left[\frac{4}{z-J}-\frac{10}{z-2J}\right].$$

2. Honeycomb

Figure 2 shows two different classes, $|\omega_1\rangle$ and $|\omega_2\rangle$, for the honeycomb lattice. For these states eigenvalues of L_0 are $3J$ and $4J$, and the numbers of spin configurations are $8(3N/2)$ and $[(3N/2)-13](3N/2)$, respectively. Therefore,

$$M^{(2)}(z)=(J/2)^4(3N/2)\left[\frac{16}{z-3J}-\frac{26}{z-4J}\right].$$

3. Simple cubic

There are three different classes of $H_I^2|\phi_0\rangle$. We show them in Fig. 3. The eigenvalues of L_0 are $8J$, $9J$, and $10J$ for $|\omega_1\rangle$, $|\omega_2\rangle$, and $|\omega_3\rangle$, respectively. Since the numbers of spin configurations, in order of states, are $4(3N)$, $2(3N)$, and $(3N-57)3N$,

$$M^{(2)}(z)=(J/2)^4(3N)\left[\frac{16}{z-8J}+\frac{84}{z-9J}-\frac{114}{z-10J}\right].$$

4. Body-centered cubic

In the bcc lattice, there are also three eigenstates, which we do not show explicitly, $|\omega_1\rangle$, $|\omega_2\rangle$, and $|\omega_3\rangle$,

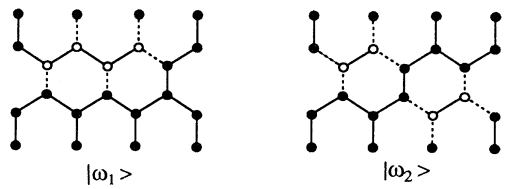

FIG. 2. Typical sign configurations of the eigenstates of L_0 in a honeycomb. Black and white dots have the same meaning as in Fig. 1.

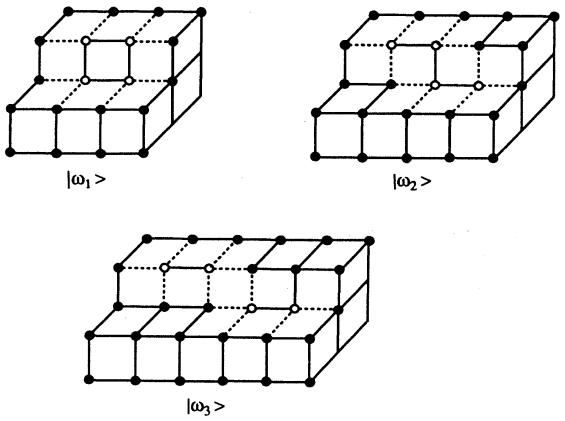

FIG. 3. Typical spin configurations of the eigenstates of L_0 in a simple cubic. Black and white dots have the same meaning as in Fig. 1.

for which the eigenvalues of L_0 are $12J$, $13J$, and $14J$, respectively. Since the numbers of spin configurations are $12(4N)$, $74(4N)$, and $(4N-101)(4N)$,

$$M^{(2)}(z)=(J/2)^4(4N)\left[\frac{48}{z-12J}+\frac{148}{z-13J}-\frac{202}{z-14J}\right].$$

APPENDIX B: $M^{(3)}(0)$ FOR THE HONEYCOMB LATTICE

Since there are two eigenstates of L_0 for the spin configuration $H_I^2|\phi_0\rangle$ in a honeycomb lattice, we choose $|A_i)$ of Eq. (15) such as $|A_0)=|H_I^2)$ and $|A_1)=L_0|H_1^2)$. By introducing μ_n as $\mu_n=(H_I^2|L_0^n H_I^2)$ for our convenience, we can simply write the matrices $\tilde{P}$ and $\tilde{\Omega}$ as follows:

$$\tilde{P}=\begin{bmatrix}\mu_0 & \mu_1\\ \mu_1 & \mu_2\end{bmatrix}=\left[\frac{J}{2}\right]^4\left[\frac{3N}{2}\right]\begin{bmatrix}-10 & -56J\\ -56J & 272J^2\end{bmatrix}$$

and

$$\tilde{\Omega}=\begin{bmatrix}\mu_1 & \mu_2\\ \mu_2 & \mu_3\end{bmatrix}=\left[\frac{J}{2}\right]^4\left[\frac{3N}{2}\right]\begin{bmatrix}-56J & -272J^2\\ -272J^2 & -1232J^3\end{bmatrix},$$

where use of $\mu_n=(J/2)^2(3N/2)[16(3J)^n-26(4J)^n]$ has been made for the honeycomb lattice.

The approximated memory matrix $\tilde{M}^{(0)}$ of Eq. (14) is obtained by setting $L=L_0$ in Eq. (15). The matrix elements $\tilde{M}_{ij}'^{(0)}(z)$ denote the matrix elements of (15) under this approximation. In fact, $\tilde{M}_{ij}'^{(0)}(z)$ is composed of three nonvanishing parts such that

$$\tilde{M}_{ij}'^{(0)}(z)=K_{ij}(z)+L_{ij}(z)+N_{ij}(z),$$

where

$$K_{ij}(z)=\left(A_i\left|H_I^\dagger\frac{1}{z-L_0}H_I A_j\right.\right),$$

$$L_{ij}(z)=\left(A_i\left|H_I\frac{1}{z-L_0}H_I^\dagger A_j\right.\right),$$

$$N_{ij}(z)=-\left[\frac{1}{z-J(q-1)}\right]\frac{(A_i|H_I^2)(H_I^2|A_j)}{(H_I|H_I)}.$$

After some calculations we obtain the following results:

$$K_{00}(z)=(J/2)^6(3N/2)\times\left[\frac{48}{z-3J}+\frac{792}{z-4J}-\frac{2952}{z-5J}+\frac{2484}{z-6J}\right],$$

$$L_{00}(z)=(J/2)^6(3N/2)\left[\frac{100}{z-2J}\right],$$

$$N_{00}(z)=-(J/2)^6(3N/2)\left[\frac{100}{z-2J}\right],$$

$$K_{10}(z)=K_{01}(z)=(J/2)^7(3N/2)\times\left[\frac{288}{z-3J}+\frac{5280}{z-4J}-\frac{21\,648}{z-5J}+\frac{19\,872}{z-6J}\right],$$

$$L_{10}(z)=L_{01}(z)=(J/2)^7(3N/2)\frac{1120}{z-2J},$$

$$N_{10}(z)=N_{01}(z)=-L_{10}(z),$$

$$K_{11}(z)=(J/2)^8(3N/2)\times\left[\frac{1728}{z-3J}+\frac{35\,200}{z-4J}-\frac{158\,752}{z-5J}+\frac{158\,976}{z-6J}\right],$$

$$L_{11}(z)=(J/2)^8(3N/2)\frac{12\,544}{z-2J}=-N_{11}(z).$$

Using these results, we obtain

$$\tilde{M}_{00}'^{(0)}(z=0)=-\tfrac{94}{5}(J/2)^5(3N/2),$$

$$\tilde{M}_{10}'^{(0)}(z=0)=\tilde{M}_{01}^{(0)}(z=0)=-\tfrac{996}{5}(J/2)^6(3N/2),$$

$$\tilde{M}_{11}'^{(0)}(z=0)=-\tfrac{10304}{5}(J/2)^7(3N/2).$$

Then the matrix $\tilde{M}'^{(0)}(0)$ is given by

$$\tilde{M}'^{(0)}(0)=(J/2)^4(3N/2)\begin{bmatrix}-9.4J & -49.8J^2\\ -49.8J^2 & -257.6J^3\end{bmatrix}.$$

Now it is easy to calculate the third-order memory function, which is the matrix element $\tilde{M}_{00}^{(0)}(0)$. Our result for $M^{(3)}(0)$ is

$$M^{(3)}(0)=(0.518\,44)(J/2)^3(3N/2).$$

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