Dynamic equations for three different qudits in a magnetic field

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Abstract

A closed system of equations for the local Bloch vectors and spin correlation functions of three magnetic qudits, which are in an arbitrary, time-dependent, external magnetic field, is obtained using decomplexification of the Liouville-von Neumann equation. The algorithm of the derivation of the dynamic equations is presented. In the basis convenient for the important physical applications structure constants of algebra su(2S+1) are calculated.

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I. INTRODUCTION

At present it is not known which experiment will lead to the reliable, prototypical quantum computing device. Quantum systems with two states, called qubits, are taken to be the basic unit for quantum information processing. The quantum systems realised on coupled qubits are widely investigated for the purpose of creation of a quantum computer. In the same time there is a possibility to solve this problem, using the systems consisting from coupled qudits (multilevel systems). Qudits possess a number of properties which differ from properties qubits and may have advantages for quantum information processing. For example, two qutrits can be entangled more strongly than two qubits [1]. The main purpose of this study is the derivation of dynamic equations for three qudit system, which is placed in a magnetic field, for entanglement study [2] and other applications. The article is organized as follows. Section II contains the model Hamiltonian including the three-particle interactions. In section III the Liouville-von Neumann equation for the matrix density of three qudits in the variable magnetic field is obtained in the Bloch’s representation in terms of local vectors and spin correlation functions taking into account three-particle interactions. We describe conservation laws which control numerical calculations effectively. The Appendix describes the Hermitian basis and analytic formulas for structure constants.

II. MODEL HAMILTONIAN

The Hamiltonian of three coupled different qudits (particles with spin 1/2, 1, 3/2, 2, . . .) in the external ac magnetic field $\mathbf{h} = (h_1, h_2, h_3)$, where $h_1, h_2, h_3$ are the Cartesian components of the external magnetic field, we will present in a form of decomposition on a complete set orthogonal Hermitian matrices $C_\alpha$, operating in the Hilbert space of three qudits $H^{S_1} \otimes H^{S_2} \otimes H^{S_3}$ with $(2S_1 + 1)(2S_2 + 1)(2S_3 + 1)$ dimension

$$\hat{H} = \frac{1}{2} h_{\sigma \tau} C^{S_1}_\sigma \otimes C^{S_2}_\sigma \otimes C^{S_3}_\tau,$$

(1)

where $S_1, S_2, S_3$ are qudit spins, $\otimes$ - denotes a direct product. $C^{S_1}_\sigma, C^{S_2}_\sigma, C^{S_3}_\tau$ are the Hermitian matrices operating in spaces $H^{S_1}, H^{S_2}, H^{S_3}$ accordingly (see Appendix). The functions $h_{\sigma \tau}$ contain one-, two- and three-qudit interactions [3], [4], [5].
III. DECOMPLEXIFICATION OF THE LIOUVILLE-VON NEUMANN EQUATION

The Liouville-von Neumann equation for the density matrix $\rho$, describing the dynamics of a 3-qudit system, has the form

$$i\partial_t \rho = [\hat{H}, \rho]$$

$$\rho(0) = \rho_0, \rho^+ = \rho, \text{ Tr } \rho = 1. \tag{2}$$

It is convenient to rewrite the equation Eq. (2) having presented the density matrix $\rho$ as well as the Hamiltonian $\hat{H}$, in the form of decomposition on a complete set orthogonal Hermitian matrices $C_\alpha$

$$\rho = \frac{1}{c_1(2S_1 + 1)c_2(2S_2 + 1)c_3(2S_3 + 1)} R_{\alpha\beta\gamma} C^{S_1}_\alpha \otimes C^{S_2}_\beta \otimes C^{S_3}_\gamma, \tag{3}$$

where $c_{1,2,3} = \sqrt{\frac{S_1(2S_1+1)}{3}}$. We define the three coherence Bloch vectors $R_{m00}, R_{0n0}, R_{00p}$, which are widely used in the theory of magnetic resonance characterize the local properties of the individual qudits,

$$c_1 c_2 c_3 R_{m00} = \text{ Tr } \rho C^{S_1}_m \otimes C^{S_2}_0 \otimes C^{S_3}_0, \tag{4a}$$

$$c_1 c_2 c_3 R_{0n0} = \text{ Tr } \rho C^{S_1}_0 \otimes C^{S_2}_n \otimes C^{S_3}_0, \tag{4b}$$

$$c_1 c_2 c_3 R_{00p} = \text{ Tr } \rho C^{S_1}_0 \otimes C^{S_2}_0 \otimes C^{S_3}_p, \tag{4c}$$

while the tensors $R_{mn0}, R_{m0p}, R_{0np}, R_{mn0}$

$$c_1 c_2 c_3 R_{mn0} = \text{ Tr } \rho C^{S_1}_m \otimes C^{S_2}_n \otimes C^{S_3}_0, \tag{5a}$$

$$c_1 c_2 c_3 R_{m0p} = \text{ Tr } \rho C^{S_1}_m \otimes C^{S_2}_0 \otimes C^{S_3}_p, \tag{5b}$$

$$c_1 c_2 c_3 R_{0np} = \text{ Tr } \rho C^{S_1}_0 \otimes C^{S_2}_n \otimes C^{S_3}_p, \tag{5c}$$

$$c_1 c_2 c_3 R_{mn0} = \text{ Tr } \rho C^{S_1}_m \otimes C^{S_2}_n \otimes C^{S_3}_0, \tag{5d}$$

describe the spin correlations. In the formulas Eq. (4), Eq. (5) $C^{S_i}_{0,\alpha} \equiv E_{S_i}$, $E_{S_i}$ is the unit matrix in dimension $(2S_i + 1)$ and each of the Latin indices designates a set of matrices $C^{S_i}_{k^i, q^{S_i}, z}$, where $1 \leq k^{S_i} \leq 2S_i$, and $1 \leq q^{S_i} \leq k^{S_i}$ in $C^{S_i}_{k^i, q^{S_i}, z}$, $C^{S_i}_{k^i, q^{S_i}, y}$ and $1 \leq k^{S_i} \leq 2S_i$, in $C^{S_i}_{k^i, z}$ in steps of $1$, $i = 1, 2, 3$.

Let’s formulate the linear algorithm of a decomplexification of the Liouville-von Neumann
This algorithm is easy to apply for the system of more than 3 qudits.

1. Insert the Hamiltonian Eq. (1) and the density matrix Eq. (3), decomposed on Hermitian basis into the Liouville-von Neumann equation Eq. (2).

2. Multiply the Liouville-von Neumann equation by all elements of the basis $C_\alpha^S_1 \otimes C_\beta^S_2 \otimes C_\gamma^S_3$ in turn.

3. Execute operation of a trace taking for each equation.

4. Apply the formula $\text{Tr} (C_\alpha^S_1 \otimes C_\beta^S_2 \otimes C_\gamma^S_3)(C_\epsilon^S_1 \otimes C_\zeta^S_2 \otimes C_\sigma^S_3)(C_\eta^S_1 \otimes C_\theta^S_2 \otimes C_\phi^S_3) = \text{Tr} C_\alpha^S_1 C_\beta^S_1 C_\gamma^S_1 \text{Tr} C_\beta^S_2 C_\eta^S_2 \text{Tr} C_\gamma^S_3 C_\theta^S_3 C_\phi^S_3$.

5. Express a trace from the three matrices through structure constants according to formulas Eqs. (A4, A5).

6. As a result the use of the structure constants symmetry the real terms in each equation are cancelled out, and the purely imaginary terms are duplicated.

7. The imaginary unit $i$ is cancelled.

This algorithm is easy to apply for the system of more than 3 qudits.

In terms of the functions $R_{\alpha\beta\gamma}$ the Liouville-von Neumann equation becomes real and comprises a closed system of first-order differential equations for the local Bloch vectors and spin correlation functions

\[ \partial_t R_{mnp} = c_2 c_3 \epsilon_{jim}^S \left( h_{j00} R_{i00} + h_{jk0} R_{i0k} + h_{j0k} R_{i0k} + h_{jk0} R_{i0k} \right), \quad (6a) \]

\[ \partial_t R_{m0n} = c_1 c_3 \epsilon_{k0n}^S \left( h_{000} R_{n0k} + h_{j00} R_{n0k} + h_{00j} R_{n0k} + h_{jir} R_{jkr} \right), \quad (6b) \]

\[ \partial_t R_{00p} = c_1 c_2 \epsilon_{ijp}^S \left( h_{00i} R_{00j} + h_{k0i} R_{k0j} + h_{00i} R_{k0j} + h_{l0i} R_{l0j} \right), \quad (6c) \]

\[ \partial_t R_{mn0} = c_2 c_3 \epsilon_{jim}^S h_{j00} R_{i0n} + c_1 c_3 \epsilon_{jkn}^S h_{0j0} R_{m0k} + c_2 c_3 \epsilon_{jim}^S h_{j0n} R_{i00} + c_1 c_3 \epsilon_{qkn}^S h_{mq0} R_{00k} + c_3 (e_{jim}^S g_{qn}^S + g_{jim}^S e_{qn}^S) h_{j00} R_{ik0} + c_2 c_3 \epsilon_{jim}^S h_{j0q} R_{mqk} + c_1 c_3 \epsilon_{jkn}^S h_{0j0} R_{mkq} + c_2 c_3 \epsilon_{jim}^S h_{j0n} R_{ikq} + c_3 (e_{jim}^S g_{kn}^S + g_{jim}^S e_{kn}^S) h_{j0q} R_{jkq}, \quad (6d) \]

\[ \partial_t R_{0mp} = c_2 c_3 \epsilon_{jim}^S h_{j00} R_{i0p} + c_1 c_2 \epsilon_{k0p}^S h_{00k} R_{m0q} + c_2 c_3 \epsilon_{jim}^S h_{j0p} R_{i00} + c_1 c_2 \epsilon_{q0p}^S h_{mq0} R_{00q} + c_3 (e_{jim}^S g_{0q}^S + g_{0q}^S e_{im}^S) h_{j00} R_{ikq} + c_2 c_3 \epsilon_{jim}^S h_{j0q} R_{mkq} + c_1 c_2 \epsilon_{q0p}^S h_{mkq} R_{00q} + c_2 c_3 \epsilon_{jip}^S h_{j0q} R_{ikp} + c_1 c_2 \epsilon_{q0p}^S h_{00q} R_{mkq} + c_3 (e_{jim}^S g_{r0}^S + g_{jim}^S e_{r0}^S) h_{j0q} R_{jkq}, \quad (6e) \]
The equations for the reduced matrices are not closed.

Reduced matrix $\mathbf{S}$ are obtained. The square polynomials also control the signs $\rho$. States in the environment of two other qudits are described by the algebraically independent \[6\]. From the conservation of purity, for which $(\rho^2)_{ik} \equiv (\rho)_{ik}$, the polynomial (square-law) invariants are obtained. The square polynomials also control the signs $R_{\alpha\beta\gamma}$. In the external dc field the energy of system is the constant:

$$E = \text{Tr} \hat{H} \rho.$$ \[7\]

Unitary evolution preserves the length of the generalized Bloch vector $b^{S_1S_2S_3}$

$$b^{S_1S_2S_3} = \sqrt{R_{m00}^2 + R_{0n0}^2 + R_{00p}^2 + R_{mn0}^2 + R_{m0p}^2 + R_{0np}^2 + R_{mmn}^2}.$$ \[8\]

The qudit with $(2S_1 + 1)$ states in the environment of two other qudits is described by the reduced matrix $\rho^{S_1}$

$$\rho^{S_1} = \frac{1}{c_1(2S_1 + 1)} (R_{000} C_0^{S_1} + R_{m00} C_m^{S_1}),$$ \[9\]

in which $R_{000} \equiv 1$, and functions $R_{m00}$ are determined by the system solution Eq. \[6\], as the equations for the reduced matrices are not closed.

For two different coupled qudits we have $\hat{H} = \frac{1}{2} h_{\alpha\beta} C_\alpha^{S_1} \otimes C_\beta^{S_2}$,

$$\rho = \frac{1}{c_1(2S_1 + 1)c_2(2S_2 + 1)} R_{\gamma\delta} C_\gamma^{S_1} \otimes C_\delta^{S_2}, \quad R_{00} = 1.$$ \[10\]
The dynamic equation Eq. (2) for two different qudits takes on the real form in terms of the functions $R_{m0}$, $R_{0m}$, $R_{mn}$ as a closed system of differential equations Eqs. (11,12,13) for the set of initial conditions:

\[
\begin{align*}
\partial_t R_{m0} &= c_2 e^{S_1}_{pim} (h_{p0}R_{i0} + h_{pt}R_{it}), \\
\partial_t R_{0m} &= c_1 e^{S_2}_{pim} (h_{0p}R_{0i} + h_{lp}R_{li}), \\
\partial_t R_{mn} &= e^{S_1}_{pin} \left[ c_2 (h_{pn}R_{i0} + h_{p0}R_{in}) + g_{rln} h_{rp}R_{il} \right] + e^{S_2}_{pin} \left[ c_1 (h_{mp}R_{0i} + h_{0p}R_{mi}) + g_{rln} h_{rp}R_{li} \right],
\end{align*}
\]

(11,12,13)

where by definition

\[
\text{Tr} \, \rho C^{S_1}_\alpha \otimes C^{S_2}_\beta = c_1 c_2 R_{\alpha\beta}.
\]

(14)

The functions $R_{m0}$, $R_{0m}$ describe the individual qudits and the functions $R_{mn}$ define their correlations. The Liouville-von Neumann equation for one qudit takes on the real form in terms of the functions $R_j$ as a closed system of differential equations:

\[
\partial_t R_l = e^{S_1}_{ijl} h_i R_j.
\]

(15)

The set of equations for 3 qubits has been obtained in [8].

The set of equations Eq. (16) with the initial conditions has wide applications, since the magnetic field enters in the form of arbitrary functions. It allows to make numerical calculations for continuous (a paramagnetic resonance in a continuous mode), as well as for pulse modes (a nuclear magnetic resonance). By means of this system it is possible to investigate the entanglement dynamics of qudits in a magnetic field as the entanglement measures are expressed in terms of the reduced density matrices or of populations. Another important application of the system Eq. (6) is quantum approach to the Carnot cycle [9], [10], [11], [12], [13], when a working body is a finite spin chain.

IV. CONCLUSION

The simple algorithm of the derivation of equation system for coupled qudits, which are in an arbitrary, time-dependent external magnetic field has been presented. It is not
necessary for the basis to be Hermitian since the results of calculations are independent of the choice of base, but there is the main advantage with the Hermitian basis. It is that the Liouville-von Neuman equation not involve any complex numbers and can be solved using real algebra. This is not true for non-Hermitian bases. Real algebra makes numerical calculations faster and simplifies the interpretation of the equation system Eqs. (6).

This basis forms a natural basis for calculations on coupled spin systems [14] because all the single-spin operators are part of the complete basis when the unit operator is part of the single-spin basis.

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APPENDIX A

Let \( \{C^S_1, C^S_2, ..., C^S_n\} \) be a base of su(2S+1) algebra, where \( S = 1/2, 1, 3/2, ... \) is the spin quantum number, \( n = (2S + 1)^2 - 1 \). We have according to [15]

\[
C^S_i C^S_j = \frac{c}{d} E \delta_{ij} + z^S_{ijk} C^S_k, \quad \text{Tr} C^S_i = 0, \quad \text{Tr} C^S_i C^S_j = c \delta_{ij},
\]

(A1)

\[
z^S_{ijk} = g^S_{ijk} + i e^S_{ijk},
\]

(A2)

hence

\[
- i[C^S_i, C^S_j] = 2e^S_{ijk} C^S_k, \quad \{C^S_i, C^S_j\} = \frac{c}{d} E \delta_{ij} + 2g^S_{ijk} C^S_k,
\]

(A3)

\[
e^S_{ijk} = \frac{1}{2ic} \text{Tr} [C^S_i, C^S_j] C^S_k,
\]

(A4)

\[
g^S_{ijk} = \frac{1}{2c} \text{Tr} \{C^S_i, C^S_j\} C^S_k,
\]

(A5)

where \( d = 2S + 1 \), \( E \) is the unit matrix in dimension \( d \times d \), \( c \) is a constant, \( \text{Tr} \) is a symbol for trace. It is easy to see that the structure constants \( e^S_{ijk} \) and \( g^S_{ijk} \) are completely antisymmetric and symmetric in the displacement of any pair of indices.
1. Hermitian basis

The structure constants of $su(2S + 1)$ algebra have important physical applications. In order to calculate the structure constants we have to choose the basis. The basis is based on linear combinations of irreducible tensor operators. The matrix representations of irreducible tensor operators $T_{k,q}^S \[16\]$ can be calculated using the Wigner $3jm$ symbols:

$$T_{k,q}^S = \sqrt{(2S + 1)(2k + 1)} \sum_{m,m'=-S}^S (-1)^{S-m} \binom{S}{m,m'} (-q k, S) |S,m><S,m'|,$$  \hspace{1cm} (A6)

where $0 \leq k \leq 2S$, and $-k \leq q \leq k$ in steps of 1. The normalization is such that $T_{0,0}^S = E$.

It is known that the Cartesian product operators $S_x, S_y, \text{ and } S_z$ for spin $S = \frac{1}{2}$ are Hermitian and can be calculated from irreducible tensor operators \[17\]

$$S_x^\frac{1}{2} = \frac{1}{2\sqrt{2}} (T_{\frac{1}{2},-1}^\frac{1}{2} - T_{\frac{1}{2},1}^\frac{1}{2}) = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$  \hspace{1cm} (A7a)

$$S_y^\frac{1}{2} = \frac{i}{2\sqrt{2}} (T_{\frac{1}{2},-1}^\frac{1}{2} + T_{\frac{1}{2},1}^\frac{1}{2}) = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$  \hspace{1cm} (A7b)

$$S_z^\frac{1}{2} = \frac{1}{2} T_{\frac{1}{2},0}^\frac{1}{2} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \hspace{1cm} (A7c)$$

Allard and Härd \[14\] have formed linear combinations of the irreducible tensor operators not only for single-quantum coherences, but also for all coherences according to

$$C_{k,qx}^S = \sqrt{\frac{S(S+1)}{6}} (T_{k,-q}^S + (-1)^q T_{k,q}^S), \quad q \neq 0,$$  \hspace{1cm} (A8a)

$$C_{k,qy}^S = i \sqrt{\frac{S(S+1)}{6}} (T_{k,-q}^S - (-1)^q T_{k,q}^S), \quad q \neq 0,$$  \hspace{1cm} (A8b)

$$C_{k,z}^S = \frac{1}{3} T_{k,0}^S, \quad q = 0, k \geq 1,$$  \hspace{1cm} (A8c)

$$C_{0,z}^S = \sqrt{\frac{S(S+1)}{3}} E,$$  \hspace{1cm} (A9)

where $1 \leq k \leq 2S$, and $1 \leq q \leq k$ in $C_{k,qx}^S, C_{k,qy}^S$ and $1 \leq k \leq 2S$, in $C_{k,z}^S$ in steps of 1. The matrices Eqs. (A8) are traceless and their number is equal to $(2S + 1)^2 - 1$. Using the well-known relations for the irreducible tensor operators

$$(T_{k,q}^S)^\dagger = (-1)^q T_{k,-q},$$  \hspace{1cm} (A10)
we can see that matrices Eqs. (A8) are Hermitian. Using the formula from [16]

\[ \text{Tr} T_{k,q}^S T_{k',q'}^S = (-1)^q(2S + 1)\delta_{k,k'}\delta_{q,-q'} \]  

(A11)

it is easy to show that the basis is normalized so that \( S_x = C_{1,x}^S, \quad S_y = C_{1,y}^S, \quad S_z = C_{1,z}^S \), irrespective of the spin quantum number \( S \), i.e.

\[ (C_r, C_s) = \text{Tr} C_r C_s = \delta_{r,s} \frac{S(S + 1)(2S + 1)}{3}. \]  

(A12)

The set Eqs. (A8-A9) is complete. The matrices \( C_{k,z} \) are diagonal

\[ [C_{k,z}^S, C_{k',z}^S] = 0. \]  

(A13)

There also exist the other useful bases [18], [19]. From the physical point of view, for important physical applications the basis [14] is preferred.

2. Analytic formulas for structure constants

There are 27 combinations in threes including the repetitions: \( XX'X'', \quad XX'Y'', \quad XX'Z'' \ldots \), where \( X = C_{k,q,x}^S, \quad X' = C_{k',q',x}^S, \quad Y'' = C_{k'',q'',y}^S, \quad Z'' = C_{k'',z}^S \) and so on. The use of the symmetrical properties of the Wigner 3\( jm \) symbols and the formula 2.4 (23) [16]

\[ \text{Tr} T_{k,q}^S T_{k',q}^S T_{k'',q''}^S = (-1)^{2S+k+k'+k''}(2S + 1)^{\frac{3}{2}} \]

\[ [(2k+1)(2k'+1)(2k''+1)]^{\frac{1}{2}} \{ \{ \frac{S}{S} \} \{ k \{ k' k'' \} \{ S \} S \} S \} \]

(A14)

where \( \{ \frac{k}{S} S \} \) is the 6\( j \) symbol, allows us after substitution of Eqs. (A8) in Eq. (4), Eq. (5) , to calculate all structure constants of \( su(2S + 1) \) algebra. Let us introduce the function

\[ F(k, k', k'', S) = \frac{(-1)^{2S}}{\sqrt{3}} \sqrt{S(S + 1)(2S + 1)} \times \frac{1}{(2k+1)(2k'+1)(2k''+1)} \{ \{ \frac{k}{S} S \} \{ k' \{ k'' \} S \} S \}. \]  

(A15)

All antisymmetric structure constants are zero for \( K = k + k' + k'' \) even and nonvanishing antisymmetric structure constants in terms of 3\( jm \) and 6\( j \) symbols have the explicit form are presented by formulas Eqs. (A16a-A16c) for \( K \) odd:

\[ e_{XX'Y''}^S = F \left[ (-1)^q \left( \frac{k}{q} \frac{k'}{q'} \frac{k''}{q''} \right) + (-1)^q' \left( \frac{k'}{q} \frac{k''}{q'} \frac{k''}{q''} \right) + (-1)^q'' \left( \frac{k}{q} \frac{k'}{q'} \frac{k''}{q''} \right) \right], \]  

(A16a)

\[ e_{YY'Y''}^S = F \left[ (-1)^q \left( \frac{k}{q} \frac{k'}{q'} \frac{k''}{q''} \right) + (-1)^q' \left( \frac{k'}{q} \frac{k''}{q'} \frac{k''}{q''} \right) + (-1)^q'' \left( \frac{k}{q} \frac{k'}{q'} \frac{k''}{q''} \right) \right], \]  

(A16b)
\[ e_{XY'Z''}^S = -F(-1)^q \left( \frac{k k' k''}{q - q' - q''} \right). \] (A16c)

All symmetric structure constants are zero for \( K = k + k' + k'' \) odd and nonvanishing symmetric structure constants in terms of \( 3jm \) and \( 6j \) symbols have the explicit form are presented by formulas Eqs. (A17a, A17b, A17c) for \( K \) even:

\[ g_{XX'X''}^S = \frac{F}{\sqrt{2}} \left[ (-1)^q \left( \frac{k k' k''}{q - q' - q''} \right) + (-1)^q \left( \frac{k k' k''}{q - q' - q''} \right) + (-1)^q \left( \frac{k k' k''}{q - q' - q''} \right) \right], \] (A17a)

\[ g_{XY'Y''}^S = \frac{F}{\sqrt{2}} \left[ (-1)^q \left( \frac{k k' k''}{q - q' - q''} \right) + (-1)^q \left( \frac{k k' k''}{q - q' - q''} \right) + (-1)^q \left( \frac{k k' k''}{q - q' - q''} \right) \right], \] (A17b)

\[ g_{X'X''Z'}^S = g_{Y'Y''Z'}^S = F(-1)^q \left( \frac{k k' k''}{q - q' - q''} \right), \] (A17c)

We have in \( X, Y, 1 \leq k, k', k'' \leq 2S, 1 \leq q \leq k, 1 \leq q' \leq k', 1 \leq q'' \leq k'' \) and in \( Z \) \( 1 \leq k, k', k'' \leq 2S \) in steps of 1.

The straightforward calculation confirms that the structure constants \( e_{ijk}^S \) and \( g_{ijk}^S \) are completely antisymmetric and symmetric in the displacement of any pair of operators. In other words it is \( e_{XX'Y''}^S = -e_{XY'X''}^S, g_{XX'Z''}^S = g_{Y'Y''Z'}^S \) and so on.
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