Sum rules for spin-1/2 quantum gases in states with well-defined spins. II. Spin-dependent two-body interactions

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Sums of matrix elements of spin-dependent two-body momentum-independent interactions and sums of their products are calculated analytically in the basis of many-body states with given total spin—the states built from spin and spatial wave functions belonging to multidimensional irreducible representations of the symmetric group, unless the total spin has the maximal allowed value. As in the first part of the series [V. A. Yurovsky, Phys. Rev. A **91**, 053601 (2015)], the sum dependence on the many-body states is given by universal factors, which are independent of the Hamiltonians of noninteracting particles. The sum rules are applied to perturbative analysis of energy spectra and to calculation of two-body spin-dependent local correlations.

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I. INTRODUCTION

The present paper continues analyses (see Ref. [1] for a more comprehensive introduction and definitions) of the sum rules for many-body systems of indistinguishable spin-$\frac{1}{2}$ particles. The particles can be composite, e.g., atoms or molecules, and the spin can be either a real angular momentum of the particle or a formal spin, whose projections are attributed to the particle's internal states (e.g., hyperfine states of atoms). In the latter case, the spin $\frac{1}{2}$ means that only two internal states are present in the system. This formal spin is not related to the real, physical, spin of the particles, which can be either bosons or fermions.

The many-body wave functions are represented here, as well as in [1], as a sum of products of the collective spin and spatial functions. These functions depend on spin projections and coordinates, respectively, of all particles and belong to multidimensional, non-Abelian representations of the symmetric group (see [2–5]), unless the total spin has the maximal allowed value. For spin-$\frac{1}{2}$ particles, the representation is unambiguously determined by the total many-body spin. This approach is applicable to the Hamiltonians which are separable to spin-independent and coordinate-independent parts. It differs from the conventional approach (see [6] and [1]), where each particle is characterized by its spin projection and coordinate, and the total wave function is symmetrized for bosons or antisymmetrized for fermions over permutations of all particles. The total many-body spin is undefined in this case. As follows from the Heitler's results [7] (see also [1]), an exact wave function for particles with spin-independent interactions cannot be obtained in the approach with defined individual spin projections. Many-body states with defined total spin [8–15], including the collective spin and spatial wave functions [16–19], were applied to spinor quantum gases (see [20–30]). Such states were also proposed for implementation of permutation quantum computers [31]. Other kings of entangled states with nontrivial symmetry have been analyzed for quantum-degenerate gases of spin-1 [32] and spin-2 [33] bosons. A more comprehensive review is presented in Ref. [1].

The well-known mean-field approach (see [6,24]), where the interactions between particles are replaced by the self-consistent field, is generally applied to states with defined individual spin projections and undefined total spins. It can be applied to certain states with defined total spins if the interactions are spin independent. For bosons, the many-body mean-field wave function contains a single spatial orbital, determined by the Gross-Pitaevskii equation (see [24]). For fermions, the Hartree-Fock wave function (see [6]) contains double-occupied spatial orbitals. Such wave functions have the total spin $S=N/2$ or $S=0$ for N spin-$\frac{1}{2}$ bosons or fermions, respectively, and describe quantum-degenerate gases with multiple occupations of the spatial orbitals. The present approach describes states with arbitrary total spins and is suitable for nondegenerate gases.

For spin-independent two-body interactions between particles, sums of matrix elements directly follow from Heitler's results [7], while the sum of the matrix element squared moduli was calculated in [1]. Matrix elements of spin-dependent interactions depend on the total spin projections of the coupled many-body states. For spin-dependent one-body interactions with external fields, this dependence was factorized using the Wigner-Eckart theorem and sums of the matrix elements and their squared moduli were calculated [1].

The present work is devoted to spin-dependent two-body interactions between particles. As well as in Ref. [1], the matrix elements are calculated in the basis of noninteracting particles with single occupation of spatial modes. The interactions are expressed in terms of irreducible spherical tensors and their matrix elements are related to ones for the maximal allowed projections of the total spins using the Wigner-Eckart theorem in Sec. II. Sums of these matrix elements and their squared moduli are calculated in Sec. III for zero-range spin-dependent interactions. The sum rules are applied to perturbative analysis of energy spectra in Sec. IV. Average two-body spin-dependent correlations are analyzed in this section too. These correlations allow us to distinguish between the many-body states with defined total spins and individual spin projections. Appendixes contain the calculation of sums, used in Sec. III.

References to equations in the previous paper [1] (Paper I of this series) are referred to as "(I.x)". The present paper, as well as [1], uses the following notation for the universal factors. In the ratios of the $3j$-Wigner symbols $X_{S_z k}^{(S,S',q)}$, giving the dependence on the total spin projections, S and S' are the maximal and minimal total spins of the coupled states, q is the rank of the spherical tensor, and S_z and S_z+k are the spin projections for S and S', respectively. The factors $Y_i^{(S,m)}[\hat{A}]$ and $Y_i^{(S,m)}[\hat{A},\hat{B}]$, respectively, appear in the sum rules for the matrix elements of $\hat{A}$ and products of the matrix elements of $\hat{A}$ and $\hat{B}$ for the maximal allowed spin projections. Here $\hat{A}$ and $\hat{B}$ are arbitrary operators, S is the maximal total spin of the coupled states, and m is the number of changed spatial quantum numbers (it is omitted if the factor is independent of m). If the sum rule contains several factors Y, they are specified by the subscript i.

II. SPIN-PROJECTION DEPENDENCE

Let $|\uparrow\rangle$ and $|\downarrow\rangle$ denote two spin states of the particles. Permutation-invariant momentum-independent two-body interactions between particles with arbitrary spin dependence can be decomposed into irreducible spherical tensors of ranks 0, 1, and 2 using general relations [34] between irreducible spherical and Cartesian tensors. In the present case the Cartesian tensors are proportional to the products $\hat{s}_\alpha(j)\hat{s}_{\alpha'}(j')$ of the spin components of two particles, where α and α' can be either x, y, or z. The z component of the jth particle spin is

$$\hat{s}_z(j)=\tfrac{1}{2}(|\uparrow(j)\rangle\langle\uparrow(j)|-|\downarrow(j)\rangle\langle\downarrow(j)|), \tag{1}$$

while $\hat{s}_x(j)=\frac{1}{2}[\hat{s}_+(j)+\hat{s}_-(j)]$ and $\hat{s}_y(j)=-\frac{i}{2}[\hat{s}_+(j)-\hat{s}_-(j)]$ are expressed in terms of the spin raising and lowering operators

$$\hat{s}_+(j)=|\uparrow(j)\rangle\langle\downarrow(j)|,\quad \hat{s}_-(j)=|\downarrow(j)\rangle\langle\uparrow(j)|.$$

There are two zero-rank tensors (spherical scalars),

$$\hat{V}=\sum_{j\neq j'}V^+(\mathbf{r}_j-\mathbf{r}_{j'}) \tag{2}$$

and

$$\hat{V}_0^{(0)}=-\frac{1}{\sqrt{3}}(\hat{V}_{zz}+\hat{V}_{+-}^+),$$

where

$$\begin{aligned}\hat{V}_{zz}&=\sum_{j\neq j'}V^+(\mathbf{r}_j-\mathbf{r}_{j'})\hat{s}_z(j)\hat{s}_z(j'),\\ \hat{V}_{+-}^+&=\sum_{j\neq j'}V^+(\mathbf{r}_j-\mathbf{r}_{j'})\hat{s}_+(j)\hat{s}_-(j').\end{aligned} \tag{3}$$

Here

$$V^\pm(\mathbf{r})=\tfrac{1}{2}[V(\mathbf{r})\pm V(-\mathbf{r})]$$

are the even and odd parts of the two-body potential function $V(\mathbf{r})$,

The three components of the rank-1 spherical tensor $\hat{V}^{(1)}$ can be expressed as

$$\begin{aligned}\hat{V}_0^{(1)}&=\frac{1}{\sqrt{2}}\sum_{j\neq j'}V^-(\mathbf{r}_j-\mathbf{r}_{j'})\hat{s}_+(j)\hat{s}_-(j'),\\ \hat{V}_{\pm1}^{(1)}&=-\sum_{j\neq j'}V^-(\mathbf{r}_j-\mathbf{r}_{j'})\hat{s}_z(j)\hat{s}_\pm(j').\end{aligned}$$

Finally,

$$\begin{aligned}\hat{V}_0^{(2)}&=\frac{1}{\sqrt{6}}(2\hat{V}_{zz}-\hat{V}_{+-}^+),\\ \hat{V}_{\pm1}^{(2)}&=\mp\sum_{j\neq j'}V^+(\mathbf{r}_j-\mathbf{r}_{j'})\hat{s}_z(j)\hat{s}_\pm(j'),\\ \hat{V}_{\pm2}^{(2)}&=\frac{1}{2}\sum_{j\neq j'}V^+(\mathbf{r}_j-\mathbf{r}_{j'})\hat{s}_\pm(j)\hat{s}_\pm(j')\end{aligned}$$

are the five components of the rank-2 spherical tensor $\hat{V}^{(2)}$. The even or odd rank tensors depend, respectively, on the even or odd components $V^\pm(\mathbf{r})$ of the potential. Therefore the rank-1 tensor vanishes in the case of even two-body interaction, while the scalars and rank-2 tensor vanish for the odd interaction.

The interactions conserving the z projection of the total many-body spin are expressed in terms of the scalars and zero components of the tensors,

$$\begin{aligned}\hat{V}_{\uparrow\uparrow}&\equiv\sum_{j\neq j'}V(\mathbf{r}_j-\mathbf{r}_{j'})|\uparrow(j)\rangle|\uparrow(j')\rangle\langle\uparrow(j)|\langle\uparrow(j')|\\ &=\sqrt{\frac{2}{3}}\hat{V}_0^{(2)}-\frac{1}{\sqrt{3}}\hat{V}_0^{(0)}+\hat{V}_0^++\frac{1}{4}\hat{V},\end{aligned} \tag{4a}$$

$$\begin{aligned}\hat{V}_{\downarrow\downarrow}&\equiv\sum_{j\neq j'}V(\mathbf{r}_j-\mathbf{r}_{j'})|\downarrow(j)\rangle|\downarrow(j')\rangle\langle\downarrow(j)|\langle\downarrow(j')|\\ &=\sqrt{\frac{2}{3}}\hat{V}_0^{(2)}-\frac{1}{\sqrt{3}}\hat{V}_0^{(0)}-\hat{V}_0^++\frac{1}{4}\hat{V},\end{aligned} \tag{4b}$$

$$\begin{aligned}\hat{V}_{\uparrow\downarrow}&\equiv\sum_{j\neq j'}V(\mathbf{r}_j-\mathbf{r}_{j'})|\uparrow(j)\rangle|\downarrow(j')\rangle\langle\uparrow(j)|\langle\downarrow(j')|\\ &=-\sqrt{\frac{2}{3}}\hat{V}_0^{(2)}+\frac{1}{\sqrt{3}}\hat{V}_0^{(0)}-\hat{V}_0^-+\frac{1}{4}\hat{V},\end{aligned} \tag{4c}$$

$$\begin{aligned}\hat{V}_{+-}&\equiv\sum_{j\neq j'}V(\mathbf{r}_j-\mathbf{r}_{j'})|\uparrow(j)\rangle|\downarrow(j')\rangle\langle\downarrow(j)|\langle\uparrow(j')|\\ &=-\sqrt{\frac{2}{3}}\hat{V}_0^{(2)}-\frac{2}{\sqrt{3}}\hat{V}_0^{(0)}+\sqrt{2}\hat{V}_0^{(1)}.\end{aligned} \tag{4d}$$

Here

$$\hat{V}_0^\pm=\sum_{j\neq j'}V^\pm(\mathbf{r}_j-\mathbf{r}_{j'})\hat{s}_z(j)$$

are zero components of spherical vectors (see [34]). Equations (4a) and (4b) lead to the relation

$$\hat{V}_0^+=\tfrac{1}{2}(\hat{V}_{\uparrow\uparrow}-\hat{V}_{\downarrow\downarrow}). \tag{5}$$

The interactions changing the spin of one of the colliding particles,

$$\begin{aligned}\hat{V}_{-\uparrow}&\equiv\sum_{j\neq j'}V(\mathbf{r}_j-\mathbf{r}_{j'})|\downarrow(j)\rangle|\uparrow(j')\rangle\langle\uparrow(j)|\langle\uparrow(j')|\\ &=\hat{V}_{-1}^{(2)}+\hat{V}_{-1}^{(1)}+\frac{1}{\sqrt{2}}\hat{V}_{-1},\\ \hat{V}_{-\downarrow}&\equiv\sum_{j\neq j'}V(\mathbf{r}_j-\mathbf{r}_{j'})|\downarrow(j)\rangle|\downarrow(j')\rangle\langle\uparrow(j)|\langle\downarrow(j')|\\ &=-\hat{V}_{-1}^{(2)}-\hat{V}_{-1}^{(1)}+\frac{1}{\sqrt{2}}\hat{V}_{-1},\end{aligned} \tag{6}$$

involve also

$$\hat{V}_{\pm 1} = \mp \frac{1}{\sqrt{2}} \sum_{j \neq j'} V(\mathbf{r}_j - \mathbf{r}_{j'}) \hat{s}_{\pm}(j),$$

which form a spherical vector together with $\hat{V}_0 = \hat{V}_z^+ + \hat{V}_z^-$ (see [34]).

The interaction

$$\hat{V}_{--} \equiv \sum_{j \neq j'} V(\mathbf{r}_j - \mathbf{r}_{j'}) |\downarrow(j)\rangle |\downarrow(j')\rangle \langle \uparrow(j)| \langle \uparrow(j')| = 2\hat{V}_{-2}^{(2)} \quad (7)$$

changes spins of both colliding particles. Other spin-changing interactions are obtained by the Hermitian conjugation of Eqs. (6) and (7), taking into account that

$$\left(\hat{V}_{-2}^{(2)}\right)^\dagger = \hat{V}_{+2}^{(2)}, \quad \left(\hat{V}_{-1}^{(2)}\right)^\dagger = -\hat{V}_{+1}^{(2)},$$
$$\left(\hat{V}_{-1}^{(1)}\right)^\dagger = \hat{V}_{+1}^{(1)}, \quad \hat{V}_{-1}^\dagger = -\hat{V}_{+1}. \quad (8)$$

Consider matrix elements between wave functions $\Psi_{nS_z}^{(S)}$ with the defined projection S_z of the total spin S. The explicit form of $\Psi_{nS_z}^{(S)}$, given by Eq. (I.16), is not used here. The multi-index n labels different functions with the same S and S_z. According to the Wigner-Eckart theorem (see [35]), the matrix elements of the spherical scalars are diagonal in spins and independent of the spin projection,

$$\langle \Psi_{n'S'_z}^{(S')} | \hat{V} | \Psi_{nS_z}^{(S)} \rangle = \delta_{SS'} \delta_{S_z S'_z} \langle \Psi_{n'S}^{(S)} | \hat{V} | \Psi_{nS}^{(S)} \rangle,$$
$$\langle \Psi_{n'S'_z}^{(S')} | \hat{V}_0^{(0)} | \Psi_{nS_z}^{(S)} \rangle = \delta_{SS'} \delta_{S_z S'_z} \langle \Psi_{n'S}^{(S)} | \hat{V}_0^{(0)} | \Psi_{nS}^{(S)} \rangle.$$

The matrix elements of the spherical vectors and the rank-1 tensor follow the same relations (I.23) as the one-body interactions,

$$\langle \Psi_{n'S'_z}^{(S')} | \hat{A}_k | \Psi_{nS_z}^{(S)} \rangle = \delta_{S'_z S_z + k} X_{S_z k}^{(S,S',1)} \langle \Psi_{n'S'}^{(S')} | \hat{A}_{S'-S} | \Psi_{nS}^{(S)} \rangle, \quad (9)$$

where the factors

$$X_{S_z k}^{(S,S',q)} = (-1)^{S'-S_z-k} \begin{pmatrix} S & S' & q \\ S_z & -S_z - k & k \end{pmatrix} \times \begin{pmatrix} S & S' & q \\ S & -S' & S' - S \end{pmatrix}^{-1}$$

are expressed in terms of the $3j$-Wigner symbols. Here $\hat{A}_0$ can be either $\hat{V}_0^{\pm}$, $\hat{V}_0$, or $\hat{V}_0^{(1)}$, and $\hat{A}_{\pm 1}$ can be $\hat{V}_{\pm 1}$, or $\hat{V}_{\pm 1}^{(1)}$. According to the properties of the $3j$-Wigner symbols, the matrix elements (9) vanish if $|S - S'| > 1$ (in agreement to the selection rules [19]). The factors $X_{S_z k}^{(S,S',1)}$ for $S' \leqslant S$ are presented in Table I in Ref. [1]. The Hermitian conjugate of Eq. (9), together with Eq. (8) and relations $(\hat{V}_0^{\pm})^\dagger = \hat{V}_0^{\pm}$, $(\hat{V}_0)^\dagger = \hat{V}_0$, and $(\hat{V}_0^{(1)})^\dagger = -\hat{V}_0^{(1)}$, give us the matrix elements for $S' = S + 1$.

The matrix elements of the components of the rank-2 spherical tensor $\hat{V}_k^{(2)}$ can be expressed in terms of the matrix elements for the maximal allowed spin projections ($S' \leqslant S$) in the same way,

$$\langle \Psi_{n'S'_z}^{(S')} | \hat{V}_k^{(2)} | \Psi_{nS_z}^{(S)} \rangle = \delta_{S'_z S_z + k} X_{S_z k}^{(S,S',2)} \langle \Psi_{n'S'}^{(S')} | \hat{V}_{S'-S}^{(2)} | \Psi_{nS}^{(S)} \rangle. \quad (10)$$

According to the properties of the $3j$-Wigner symbols, the matrix elements (10) vanish if $|S - S'| > 2$ (in agreement to the selection rules [19]). The nonvanishing factors $X_{S_z k}^{(S,S',2)}$, calculated with the $3j$-Wigner symbols [6,35], are presented in Table I. The symmetry properties of the $3j$-Wigner symbols [6,35] lead to the relation

$$X_{S_z -k}^{(S,S',q)} = (-1)^{S-S'+q} X_{-S_z k}^{(S,S',q)},$$

providing the factors $X_{S_z k}^{(S,S',2)}$ for $k < 0$. The matrix elements for $S + 1 \leqslant S' \leqslant S + 2$ are given by Hermitian conjugation of Eq. (10), taking into account Eq. (8) and the relation $(\hat{V}_0^{(2)})^\dagger = \hat{V}_0^{(2)}$.

Thus, each permutation-invariant two-body interaction between particles is expressed in terms of irreducible spherical tensors. Their matrix elements for arbitrary total spin projections are related to ones for the maximal allowed spin projections using the Wigner-Eckart theorem. The next section deals with the later matrix elements.

III. SUM RULES

A. Matrix elements for zero-range interactions

The sums of the matrix elements and sums of their squared moduli will be evaluated here for zero-range spin-dependent two-body interactions with the even potential function

$$V(\mathbf{r}) = \delta(\mathbf{r}), \quad (11)$$

where $\mathbf{r}$ is a D-dimensional vector. This function is generally used for description of interactions of cold atoms in free space, when $D = 3$, and under tight pancake- or cigar-shape confinement, when $D = 2$ or $D = 1$, respectively. In the three- and two-dimensional cases the δ function has to be properly renormalized.

For the even potential function, we have $V^+(\mathbf{r}) = V(\mathbf{r})$, $V^-(\mathbf{r}) = 0$, and, therefore, $\hat{V}_k^{(1)} = \hat{V}_0^- = 0$, $\hat{V}_{+-} = \hat{V}_{+-}^+$. Besides, the identity $|\uparrow(j)\rangle\langle\uparrow(j)| + |\downarrow(j)\rangle\langle\downarrow(j)| = 1$ leads to the relation

$$\hat{V}_{\uparrow\downarrow} = \tfrac{1}{2}(\hat{V} - \hat{V}_{\uparrow\uparrow} - \hat{V}_{\downarrow\downarrow}). \quad (12)$$

The zero range of interaction allows us to relate the matrix elements of $\hat{V}_{\uparrow\downarrow}$ and $\hat{V}_{+-}$, defined by (4c) and (4d), respectively, in the following way. Wave functions of indistinguishable particles Ψ obey to the quantum exclusion principle $\mathcal{P}_{jj'}\Psi = \pm\Psi$, where the sign $+$ or $-$ is taken for bosons or fermions, respectively. Therefore

$$\langle \Psi' | \hat{V}_{+-} | \Psi \rangle = \pm \sum_{j \neq j'} \langle \Psi' | \uparrow(j) \rangle | \downarrow(j') \rangle \delta(\mathbf{r}_j - \mathbf{r}_{j'}) \times \langle \downarrow(j) | \langle \uparrow(j') | \mathcal{P}_{jj'} | \Psi \rangle.$$

The permutation operator $\mathcal{P}_{jj'}$ permutes both spins and the coordinates $\mathbf{r}_j$ and $\mathbf{r}_{j'}$. However, the δ function sets $\mathbf{r}_j = \mathbf{r}_{j'}$ and the coordinate permutation has no effect. Acting to the left, permutation $\mathcal{P}_{jj'}$ of spins is restricted by the bra $\langle \downarrow(j) | \langle \uparrow(j') |$ of the interaction operator, therefore

$$\langle \Psi' | \hat{V}_{+-} | \Psi \rangle = \pm \sum_{j \neq j'} \langle \Psi' | \uparrow(j) \rangle | \downarrow(j') \rangle \delta(\mathbf{r}_j - \mathbf{r}_{j'}) \times \langle \downarrow(j') | \langle \uparrow(j) | \Psi \rangle = \pm \langle \Psi' | \hat{V}_{\uparrow\downarrow} | \Psi \rangle.$$

TABLE I. Coefficients $X^{(S,S',2)}_{S_z k}$ in Eq. (10).

	$S-S'$		
k	0	1	2
0	$\frac{3S_z^2-S(S+1)}{S(2S-1)}$	$-\frac{S_z}{S-1}\sqrt{3\frac{S^2-S_z^2}{S(2S-1)}}$	$\sqrt{\frac{3[(S-1)^2-S_z^2](S^2-S_z^2)}{2S(S-1)(2S-1)(2S-3)}}$
1	$-\frac{(1+2S_z)\sqrt{6(S+S_z+1)(S-S_z)}}{2S(2S-1)}$	$\frac{S+2S_z+1}{S-1}\sqrt{\frac{(S-S_z-1)(S-S_z)}{2S(2S-1)}}$	$-\sqrt{\frac{(S-S_z-2)(S-S_z-1)(S^2-S_z^2)}{S(S-1)(2S-1)(2S-3)}}$
2	$\frac{\sqrt{6(S-S_z-1)(S-S_z)(S+S_z+1)(S+S_z+2)}}{2S(2S-1)}$	$-\frac{1}{S-1}\sqrt{\frac{[S^2-(S_z+1)^2](S-S_z-2)(S-S_z)}{2S(2S-1)}}$	$\sqrt{\frac{(S-S_z-3)(S-S_z-2)(S-S_z-1)(S-S_z)}{4S(S-1)(2S-1)(2S-3)}}$

Then (4c) and (4d) for the even potential function, together with (12), lead to

$$\begin{aligned}\langle\Psi'|\hat{V}_0^{(0)}|\Psi\rangle &= -\frac{1}{4\sqrt{3}}\langle\Psi'|\hat{V}|\Psi\rangle,\\ \langle\Psi'|\hat{V}_0^{(2)}|\Psi\rangle &= \sqrt{\frac{3}{2}}\langle\Psi'|\frac{1}{2}(\hat{V}_{\uparrow\uparrow}+\hat{V}_{\downarrow\downarrow})-\frac{1}{3}\hat{V}|\Psi\rangle,\\ \langle\Psi'|\hat{V}_0|\Psi\rangle &= \frac{1}{2}\langle\Psi'|\hat{V}_{\uparrow\uparrow}-\hat{V}_{\downarrow\downarrow}|\Psi\rangle \end{aligned}\tag{13}$$

for bosons. Thus, matrix elements of scalars and zero components of the vector and tensors are expressed in terms of $\hat{V}$, $\hat{V}_{\uparrow\uparrow}$, and $\hat{V}_{\downarrow\downarrow}$. The nonzero components of the vector and tensor are obtained from (6) and (7),

$$\begin{aligned}\hat{V}_{-1}^{(2)} &= \frac{1}{2}(\hat{V}_{-\uparrow}-\hat{V}_{-\downarrow}),\\ \hat{V}_{-1} &= \frac{1}{\sqrt{2}}(\hat{V}_{-\uparrow}+\hat{V}_{-\downarrow}),\\ \hat{V}_{-2}^{(2)} &= \frac{1}{2}\hat{V}_{--}\end{aligned}\tag{14}$$

and their Hermitian conjugates.

For fermions, matrix elements of $\hat{V}_{\uparrow\uparrow}$, and $\hat{V}_{\downarrow\downarrow}$ are equal to zero, in agreement with the Pauli principle—two particles with the same spin cannot have equal coordinates. This leads to the zero matrix elements of the spherical vector and tensors. The matrix elements of the spherical scalars are related as

$$\langle\Psi'|\hat{V}_0^{(0)}|\Psi\rangle = \frac{\sqrt{3}}{4}\langle\Psi'|\hat{V}|\Psi\rangle.\tag{15}$$

The sums of the matrix elements of $\hat{V}$ and sums of their squared moduli are derived in Ref. [1]. Other relevant interactions are analyzed below.

B. Matrix elements for noninteracting bosons

Let us evaluate matrix elements of $\hat{V}_{\uparrow\uparrow}$, $\hat{V}_{\downarrow\downarrow}$, $\hat{V}_{-\uparrow}$, $\hat{V}_{-\downarrow}$, and $\hat{V}_{--}$ between wave functions

$$\tilde{\Psi}^{(S)}_{r\{n\}S_z} = f_S^{-1/2}\sum_t \tilde{\Phi}^{(S)}_{tr\{n\}}\Xi^{(S)}_{tS_z}\tag{16}$$

[see Eq. (I.17)] of noninteracting bosons with defined projection S_z of the total spin S, where f_S is the dimension of the respective irreducible representation of the symmetric group. The representations and functions within the representations, respectively, are labeled by the standard Young tableaux r and t of the shape $\lambda=[N/2+S,N/2-S]$ (see [4,5]). For bosons, the spatial functions of N noninteracting particles (I.11) are represented in the form

$$\tilde{\Phi}^{(S)}_{tr\{n\}} = \left(\frac{f_S}{N!}\right)^{1/2}\sum_{\mathcal{P}} D^{[\lambda]}_{rt}(\mathcal{P})\prod_{j=1}^{N}\varphi_{n_{\mathcal{P}j}}(\mathbf{r}_j),\tag{17}$$

where $\mathcal{P}$ are permutations of N symbols, $\varphi_n(\mathbf{r})$ are the spatial orbitals, and the relation for the Young orthogonal matrices

$$D^{[\lambda]}_{tr}(\mathcal{P}^{-1}) = D^{[\lambda]}_{rt}(\mathcal{P})\tag{18}$$

[see (I.7)] is used (see Ref. [1] for other notation). Each matrix element, e.g., the one of $\hat{V}_{\uparrow\uparrow}$, can be decomposed into the spatial and spin parts,

$$\begin{aligned}&\big\langle\tilde{\Psi}^{(S')}_{r'\{n'\}S_z'}\big|\hat{V}_{\uparrow\uparrow}\big|\tilde{\Psi}^{(S)}_{r\{n\}S_z}\big\rangle\\ &= (f_S f_{S'})^{-1/2}\sum_{t,t'}\sum_{i\neq i'}\big\langle\tilde{\Phi}^{(S')}_{t'r'\{n'\}}\big|V(\mathbf{r}_i-\mathbf{r}_{i'})\big|\tilde{\Phi}^{(S)}_{tr\{n\}}\big\rangle\\ &\quad\times\big\langle\Xi^{(S')}_{t'S_z}\big|\uparrow(i)\rangle|\uparrow(i')\rangle\langle\uparrow(i)|\langle\uparrow(i')\big|\Xi^{(S)}_{tS_z}\big\rangle\delta_{S_zS_z'}.\end{aligned}\tag{19}$$

Using Eq. (17), the spatial matrix elements can be expressed as

$$\begin{aligned}&\big\langle\tilde{\Phi}^{(S')}_{t'r'\{n'\}}\big|V(\mathbf{r}_i-\mathbf{r}_{i'})\big|\tilde{\Phi}^{(S)}_{tr\{n\}}\big\rangle\\ &= \frac{\sqrt{f_S f_{S'}}}{N!}\sum_{\mathcal{R},\mathcal{Q}} D^{[\lambda']}_{r't'}(\mathcal{Q})D^{[\lambda]}_{rt}(\mathcal{R})\\ &\quad\times\int d^D r_i d^D r_{i'}\varphi^*_{n'_{\mathcal{Q}i}}(\mathbf{r}_i)\varphi^*_{n'_{\mathcal{Q}i'}}(\mathbf{r}_{i'})V(\mathbf{r}_i-\mathbf{r}_{i'})\varphi_{n_{\mathcal{R}i}}(\mathbf{r}_i)\varphi_{n_{\mathcal{R}i'}}(\mathbf{r}_{i'})\\ &\quad\times\prod_{i'\neq i''\neq i}\delta_{n'_{\mathcal{Q}i''},n_{\mathcal{R}i''}}.\end{aligned}\tag{20}$$

The Kronecker δ symbols appear here due to the orthogonality of the spatial orbitals φ_n and the absence of equal quantum numbers in each of the sets $\{n\}$ and $\{n'\}$. Due to the δ symbols, all but two spatial quantum numbers remain unchanging. Supposing that the unchanged $n_{i''}$ are in the same positions in the sets $\{n\}$ and $\{n'\}$, one can see that the Kronecker symbols allow only $\mathcal{Q}=\mathcal{R}$ or $\mathcal{Q}=\mathcal{R}\mathcal{P}_{ii'}$. Therefore

$$\begin{aligned}&\big\langle\tilde{\Phi}^{(S')}_{t'r'\{n'\}}\big|V(\mathbf{r}_i-\mathbf{r}_{i'})\big|\tilde{\Phi}^{(S)}_{tr\{n\}}\big\rangle\\ &= \frac{\sqrt{f_S f_{S'}}}{N!}\sum_{\mathcal{R}} D^{[\lambda]}_{rt}(\mathcal{R})\big[D^{[\lambda']}_{r't'}(\mathcal{R})+D^{[\lambda']}_{r't'}(\mathcal{R}\mathcal{P}_{ii'})\big]\\ &\quad\times\langle n'_{\mathcal{R}i'}n'_{\mathcal{R}i}|V|n_{\mathcal{R}i'}n_{\mathcal{R}i}\rangle\prod_{\mathcal{R}i'\neq j''\neq\mathcal{R}i}\delta_{n'_{j''},n_{j''}},\end{aligned}\tag{21}$$

where for the zero-range potential (11) the matrix elements

$$\langle n_1' n_2' | V | n_1 n_2 \rangle = \langle n_2' n_1' | V | n_1 n_2 \rangle = \int d^D r \varphi^*_{n_1'}(\mathbf{r}) \varphi^*_{n_2'}(\mathbf{r}) \varphi_{n_1}(\mathbf{r}) \varphi_{n_2}(\mathbf{r})$$

are invariant over permutations of n_1' and n_2', as well as of n_1 and n_2.

All matrix elements are related by the Wigner-Eckart theorem to ones for the maximal allowed spin projection, $S_z' = S'$, $S_z = S$. The spinor matrix elements include projections of the spin wave-functions (I.14), derived in [36],

$$\Xi^{(S)}_{tS_z} = C_{SS_z} \sum_{\mathcal{P}} D^{[\lambda]}_{t[0]}(\mathcal{P}) \prod_{j=1}^{N/2+S_z} |\uparrow(\mathcal{P}j)\rangle \prod_{j=N/2+S_z+1}^{N} |\downarrow(\mathcal{P}j)\rangle,$$

with the normalization factor

$$C_{SS_z} = \frac{1}{(N/2+S_z)!(N/2-S)!} \sqrt{\frac{(2S+1)(S+S_z)!}{(N/2+S+1)(2S)!(S-S_z)!}}. \tag{22}$$

The projection

$$\langle \uparrow(i)|\langle \uparrow(i')|\Xi^{(S)}_{tS}\rangle = C_{SS} \sum_{\mathcal{P}} D^{[\lambda]}_{t[0]}(\mathcal{P}) \sum_{l \neq l'}^{\lambda_1} \delta_{i,\mathcal{P}l} \delta_{i',\mathcal{P}l'} \prod_{l \neq j \neq l'}^{\lambda_1} |\uparrow(\mathcal{P}j)\rangle \prod_{j=\lambda_1+1}^{N} |\downarrow(\mathcal{P}j)\rangle$$

(recall that $\lambda_{1,2} = N/2 \pm S$) can be transformed, using substitution $\mathcal{P} = \mathcal{Q}\mathcal{P}_{l\lambda_1-1}\mathcal{P}_{l'\lambda_1}$, to the form

$$\langle \uparrow(i)|\langle \uparrow(i')|\Xi^{(S)}_{tS}\rangle = C_{SS} \sum_{\mathcal{Q}} \sum_{l \neq l'}^{\lambda_1} D^{[\lambda]}_{t[0]}(\mathcal{Q}\mathcal{P}_{l\lambda_1-1}\mathcal{P}_{l'\lambda_1}) \delta_{i,\mathcal{Q}(\lambda_1-1)} \delta_{i',\mathcal{Q}\lambda_1} \prod_{j=1}^{\lambda_1-2} |\uparrow(\mathcal{Q}j)\rangle \prod_{j=\lambda_1+1}^{N} |\downarrow(\mathcal{Q}j)\rangle.$$

The permutations $\mathcal{P}_{l\lambda_1-1}$ and $\mathcal{P}_{l'\lambda_1}$ permute symbols in the first row of the Young tableau [0]. Therefore, $D^{[\lambda]}_{t[0]}(\mathcal{Q}\mathcal{P}_{l\lambda_1-1}\mathcal{P}_{l'\lambda_1}) = D^{[\lambda]}_{t[0]}(\mathcal{Q})$ [see Eq. (I.8)], the summand in the equation above is independent of l and l', and the projection can be expressed as

$$\langle \uparrow(i)|\langle \uparrow(i')|\Xi^{(S)}_{tS}\rangle = \lambda_1(\lambda_1-1) C_{SS} \sum_{\mathcal{Q}} D^{[\lambda]}_{t[0]}(\mathcal{Q}) \delta_{i,\mathcal{Q}(\lambda_1-1)} \delta_{i',\mathcal{Q}\lambda_1} \prod_{j=1}^{\lambda_1-2} |\uparrow(\mathcal{Q}j)\rangle \prod_{j=\lambda_1+1}^{N} |\downarrow(\mathcal{Q}j)\rangle.$$

The projections involved into matrix elements for other interactions are evaluated in the same way,

$$\langle \downarrow(i)|\langle \downarrow(i')|\Xi^{(S)}_{tS}\rangle = \lambda_2(\lambda_2-1) C_{SS} \sum_{\mathcal{Q}} D^{[\lambda]}_{t[0]}(\mathcal{Q}) \delta_{i,\mathcal{Q}(\lambda_1+1)} \delta_{i',\mathcal{Q}(\lambda_1+2)} \prod_{j=1}^{\lambda_1} |\uparrow(\mathcal{Q}j)\rangle \prod_{j=\lambda_1+3}^{N} |\downarrow(\mathcal{Q}j)\rangle,$$

$$\langle \uparrow(i)|\langle \downarrow(i')|\Xi^{(S)}_{tS}\rangle = \lambda_1\lambda_2 C_{SS} \sum_{\mathcal{Q}} D^{[\lambda]}_{t[0]}(\mathcal{Q}) \delta_{i,\mathcal{Q}\lambda_1} \delta_{i',\mathcal{Q}(\lambda_1+1)} \prod_{j=1}^{\lambda_1-1} |\uparrow(\mathcal{Q}j)\rangle \prod_{j=\lambda_1+2}^{N} |\downarrow(\mathcal{Q}j)\rangle.$$

In the spin matrix elements of $\hat{V}_{\uparrow\uparrow}$,

$$\langle \Xi^{(S)}_{t'S}|\uparrow(i)\rangle|\uparrow(i')\rangle\langle \uparrow(i)|\langle \uparrow(i')|\Xi^{(S)}_{tS}\rangle = [\lambda_1(\lambda_1-1)C_{SS}]^2 \sum_{\mathcal{Q}} D^{[\lambda]}_{t[0]}(\mathcal{Q}) \delta_{i,\mathcal{Q}(\lambda_1-1)} \delta_{i',\mathcal{Q}\lambda_1} \sum_{\mathcal{R}} D^{[\lambda]}_{t'[0]}(\mathcal{R}) \delta_{i,\mathcal{R}(\lambda_1-1)} \delta_{i',\mathcal{R}\lambda_1} \sum_{\mathcal{P}',\mathcal{P}''} \delta_{\mathcal{R},\mathcal{Q}\mathcal{P}'\mathcal{P}''},$$

the last Kronecker symbol appears due to orthogonality of the spin states and means that the permutations $\mathcal{R}$ and $\mathcal{Q}$ can be different by permutations of particles in the same spin state. They are the permutations $\mathcal{P}'$ of the first $\lambda_1 - 2$ symbols and $\mathcal{P}''$ of the last λ_2 ones. As the permutations $\mathcal{P}'$ and $\mathcal{P}''$ do not permute symbols between rows in the Young tableau [0], the equality $D^{[\lambda]}_{t'[0]}(\mathcal{Q}\mathcal{P}'\mathcal{P}'') = D^{[\lambda]}_{t'[0]}(\mathcal{Q})$ [see Eq. (I.8)] can be applied, leading to

$$\langle \Xi^{(S)}_{t'S}|\uparrow(i)\rangle|\uparrow(i')\rangle\langle \uparrow(i)|\langle \uparrow(i')|\Xi^{(S)}_{tS}\rangle = \lambda_1!\lambda_2!\lambda_1(\lambda_1-1) C^2_{SS} \sum_{\mathcal{Q}} D^{[\lambda]}_{t[0]}(\mathcal{Q}) D^{[\lambda]}_{t'[0]}(\mathcal{Q}) \delta_{i,\mathcal{Q}(\lambda_1-1)} \delta_{i',\mathcal{Q}\lambda_1}.$$

Let us substitute this equation and Eq. (21) into Eq. (19), perform the summation over t and t', using the relation

$$\sum_t D^{[\lambda]}_{r't}(\mathcal{P}) D^{[\lambda]}_{tr}(\mathcal{Q}) = D^{[\lambda]}_{r'r}(\mathcal{P}\mathcal{Q}), \tag{23}$$

[see Eq. (I.6)] and substitute $\mathcal{P}=\mathcal{Q}^{-1}\mathcal{R}^{-1}$, $j=\mathcal{R}i$, and $j'=\mathcal{R}i'$. Then the Kronecker symbols lead to $\mathcal{P}j=\mathcal{Q}^{-1}i=\lambda_1-1$ and $\mathcal{P}j'=\mathcal{Q}^{-1}i'=\lambda_1$. Equations

$$\mathcal{P}\mathcal{P}_{ii'}\mathcal{P}^{-1}=\mathcal{P}_{\mathcal{P}i\mathcal{P}i'} \tag{24}$$

(see [5]) and (I.8) lead then to $D^{[\lambda]}_{r'[0]}(\mathcal{R}\mathcal{P}_{ii'}\mathcal{Q})=D^{[\lambda]}_{r'[0]}(\mathcal{P}^{-1}\mathcal{Q}^{-1}\mathcal{P}_{ii'}\mathcal{Q})=D^{[\lambda]}_{r'[0]}(\mathcal{P}^{-1}\mathcal{P}_{\lambda_1\lambda_1-1})=D^{[\lambda]}_{r'[0]}(\mathcal{P}^{-1})$. Then using Eq. (18) we get

$$\langle\tilde{\Psi}^{(S')}_{r'\{n'\}S'}|\hat{V}_{\uparrow\uparrow}|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle=2\delta_{S'S}\lambda_1!\lambda_2!\lambda_1(\lambda_1-1)C^2_{SS}V^{[\lambda][\lambda]}_{r'\{n'\}r\{n\}}(\lambda_1-1,\lambda_1) \tag{25}$$

with

$$V^{[\lambda'][\lambda]}_{r'\{n'\}r\{n\}}(l,l')=\sum_{j\neq j'}\sum_{\mathcal{P}}D^{[\lambda']}_{[0]r'}(\mathcal{P})D^{[\lambda]}_{[0]r}(\mathcal{P})\delta_{l,\mathcal{P}j}\delta_{l',\mathcal{P}j'}\langle n'_jn'_{j'}|V|n_jn_{j'}\rangle\prod_{j'\neq j''\neq j}\delta_{n'_{j''},n_{j''}}. \tag{26}$$

Matrix elements of other operators are calculated in the same way,

$$\begin{aligned}
\langle\tilde{\Psi}^{(S')}_{r'\{n'\}S'}|\hat{V}_{\downarrow\downarrow}|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle&=2\delta_{S'S}\lambda_1!\lambda_2!\lambda_2(\lambda_2-1)C^2_{SS}V^{[\lambda][\lambda]}_{r'\{n'\}r\{n\}}(\lambda_1+1,\lambda_1+2),\\
\langle\tilde{\Psi}^{(S')}_{r'\{n'\}S'}|\hat{V}_{-\uparrow}|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle&=2\delta_{S'S-1}\lambda_1!\lambda_2!(\lambda_1-1)(\lambda_2+1)C_{SS}C_{S-1S-1}V^{[\lambda'][\lambda]}_{r'\{n'\}r\{n\}}(\lambda_1-1,\lambda_1),\\
\langle\tilde{\Psi}^{(S')}_{r'\{n'\}S'}|\hat{V}_{-\downarrow}|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle&=2\delta_{S'S-1}\lambda_1!\lambda_2!\lambda_2(\lambda_2+1)C_{SS}C_{S-1S-1}V^{[\lambda'][\lambda]}_{r'\{n'\}r\{n\}}(\lambda_1,\lambda_1+1),\\
\langle\tilde{\Psi}^{(S')}_{r'\{n'\}S'}|\hat{V}_{--}|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle&=2\delta_{S'S-2}\lambda_1!\lambda_2!(\lambda_2+1)(\lambda_2+2)C_{SS}C_{S-2S-2}V^{[\lambda'][\lambda]}_{r'\{n'\}r\{n\}}(\lambda_1-1,\lambda_1),
\end{aligned} \tag{27}$$

where $\lambda'=[N/2+S',N/2-S']$.

C. Sums of the matrix elements and their squares and products

For the matrix elements which are diagonal in the total spin and r, one can calculate their sums and write them out in the form

$$\begin{aligned}
&\sum_r\langle\tilde{\Psi}^{(S)}_{r\{n'\}S}|\hat{V}_a|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle\\
&=Y^{(S)}[\hat{V}_a]\frac{2f_S}{N(N-1)}\\
&\times\sum_{j<j'}\langle n'_jn'_{j'}|V|n_jn_{j'}\rangle\prod_{j'\neq j''\neq j}\delta_{n'_{j''},n_{j''}},
\end{aligned} \tag{28a}$$

where $\hat{V}_a$ is any two-body interaction, which does not change the spin projection. In each term of the sum over j and j', only two spatial quantum numbers can be changed. For the operators $\hat{V}_{\uparrow\uparrow}$ and $\hat{V}_{\downarrow\downarrow}$ the factors

$$Y^{(S)}[\hat{V}_{\uparrow\uparrow}]=2\lambda_1(\lambda_1-1),\quad Y^{(S)}[\hat{V}_{\downarrow\downarrow}]=2\lambda_2(\lambda_2-1),$$

calculated using Eqs. (25), (27), (22), (26), (23), and (18), are proportional to the numbers $\lambda_1(\lambda_1-1)$ and $\lambda_2(\lambda_2-1)$ of particle pairs with spins $\uparrow$ and $\downarrow$, respectively. For the spherical tensor components, the factors are calculated with Eq. (13),

$$Y^{(S)}[\hat{V}^{(2)}_0]=\sqrt{\frac{2}{3}}S(2S-1),\quad Y^{(S)}[\hat{V}_0]=2S(N-1). \tag{28b}$$

The sum of the matrix elements of the spin-independent interactions (I.45a) can be expressed for bosons and the zero-range potentials (11) in the form (28a) too with

$$Y^{(S)}[\hat{V}]=\tfrac{3}{2}N(N-2)+2S(S+1). \tag{28c}$$

The sums of squared moduli of the matrix elements (25) and (27) and their products are proportional to the sums of products of the functions (26), which can be expressed as

$$\begin{aligned}
&\sum_{r,r'}V^{[\lambda'][\lambda]}_{r'\{n'\}r\{n\}}(l_1,l'_1)V^{[\lambda'][\lambda]}_{r'\{n\}r\{n'\}}(l_2,l'_2)\\
&=\sum_{j_1\neq j'_1}\sum_{j_2\neq j'_2}\Sigma^{(S',S)}_{j_1j'_1j_2j'_2}(l_1,l'_1,l_2,l'_2)\langle n'_{j_1}n'_{j'_1}|V|n_{j_1}n_{j'_1}\rangle\\
&\times\prod_{j'_1\neq j''_1\neq j_1}\delta_{n'_{j''_1},n_{j''_1}}\langle n'_{j_2}n'_{j'_2}|V|n_{j_2}n_{j'_2}\rangle^*\prod_{j'_2\neq j''_2\neq j_2}\delta_{n'_{j''_2},n_{j''_2}},
\end{aligned} \tag{29}$$

where

$$\begin{aligned}
\Sigma^{(S',S)}_{j_1j'_1j_2j'_2}(l_1,l'_1,l_2,l'_2)&=\sum_{r,r'}\sum_{\mathcal{P}}D^{[\lambda']}_{[0]r'}(\mathcal{P})D^{[\lambda]}_{[0]r}(\mathcal{P})\delta_{l_1,\mathcal{P}j_1}\delta_{l'_1,\mathcal{P}j'_1}\\
&\times\sum_{\mathcal{Q}}D^{[\lambda']}_{[0]r'}(\mathcal{Q})D^{[\lambda]}_{[0]r}(\mathcal{Q})\delta_{l_2,\mathcal{Q}j_2}\delta_{l'_2,\mathcal{Q}j'_2}.
\end{aligned} \tag{30}$$

The sums of squared moduli contain different functions $\Sigma^{(S',S)}_{j_1j'_1j_2j'_2}$, namely $\Sigma^{(S,S)}_{j_1j'_1j_2j'_2}(\lambda_1-1,\lambda_1,\lambda_1-1,\lambda_1)$ for $\hat{V}_{\uparrow\uparrow}$, $\Sigma^{(S,S)}_{j_1j'_1j_2j'_2}(\lambda_1+1,\lambda_1+2,\lambda_1+1,\lambda_1+2)$ for $\hat{V}_{\downarrow\downarrow}$, $\Sigma^{(S-1,S)}_{j_1j'_1j_2j'_2}(\lambda_1-1,\lambda_1,\lambda_1-1,\lambda_1)$ for $\hat{V}_{-\uparrow}$, $\Sigma^{(S-1,S)}_{j_1j'_1j_2j'_2}(\lambda_1,\lambda_1+1,\lambda_1,\lambda_1+1)$ for $\hat{V}_{-\downarrow}$, and $\Sigma^{(S-2,S)}_{j_1j'_1j_2j'_2}(\lambda_1-1,\lambda_1,\lambda_1-1,\lambda_1)$ for $\hat{V}_{--}$. Calculation of the sums of squared moduli of the matrix elements of spherical vectors and tensors with (13) and (14) requires also sums over r and r' of the products of matrix elements. The latter sums contain $\Sigma^{(S,S)}_{j_1j'_1j_2j'_2}(\lambda_1-1,\lambda_1,\lambda_1+1,\lambda_1+2)$ for products of the matrix elements of $\hat{V}_{\uparrow\uparrow}$ by $\hat{V}_{\downarrow\downarrow}$ and $\Sigma^{(S-1,S)}_{j_1j'_1j_2j'_2}(\lambda_1-1,\lambda_1,\lambda_1,\lambda_1+1)$ for $\hat{V}_{-\uparrow}$ by $\hat{V}_{-\downarrow}$. The sums $\Sigma^{(S',S)}_{j_1j'_1j_2j'_2}$ are calculated in Appendix A.

The sums of products of matrix elements of $\hat{V}$ [expressed by (I.44) with the zero-range potential function (11)] by $\hat{V}_{\uparrow\uparrow}$

or $\hat{V}_{\downarrow\downarrow}$ are proportional to the sum

$$\sum_{r,r'} V^{[\lambda][\lambda]}_{r'\{n'\}r\{n\}}(l,l')\langle\tilde{\Psi}^{(S)}_{r\{n\}S}|\hat{V}|\tilde{\Psi}^{(S)}_{r'\{n'\}S}\rangle = \sum_{j_1\neq j_1'}\sum_{j_2\neq j_2'}\left[(N-2)!+\Sigma^{(S)}_{j_1j_1'j_2j_2'}(l,l')\right]\langle n'_{j_1}n'_{j_1'}|V|n_{j_1}n_{j_1'}\rangle \times \prod_{j_1'\neq j_1''\neq j_1}\delta_{n'_{j_1''},n_{j_1''}}\langle n'_{j_2}n'_{j_2'}|V|n_{j_2}n_{j_2'}\rangle^* \prod_{j_2'\neq j_2''\neq j_2}\delta_{n'_{j_2''},n_{j_2''}}, \tag{31}$$

where

$$\Sigma^{(S)}_{j_1j_1'j_2j_2'}(l,l') = \sum_{r,r'}\sum_{\mathcal{P}} D^{[\lambda]}_{[0]r'}(\mathcal{P})D^{[\lambda]}_{[0]r}(\mathcal{P})\delta_{l,\mathcal{P}j_1}\delta_{l',\mathcal{P}j_1'} \times D^{[\lambda]}_{rr'}(\mathcal{P}_{j_2j_2'}) \tag{32}$$

is calculated in Appendix B. Equation (31) contains $\Sigma^{(S)}_{j_1j_1'j_2j_2'}(\lambda_1-1,\lambda_1)$ and $\Sigma^{(S)}_{j_1j_1'j_2j_2'}(\lambda_1+1,\lambda_1+2)$ for $\hat{V}_{\uparrow\uparrow}$ and $\hat{V}_{\downarrow\downarrow}$, respectively. The sums of squared moduli of the matrix elements and their products are expressed in different forms if the set of spatial quantum numbers is changed ($\{n\}\neq\{n'\}$) or conserved ($\{n\}=\{n'\}$).

D. Changing set of spatial quantum numbers

If the sets of spatial quantum numbers $\{n\}$ and $\{n'\}$ are different by two elements, the product of Kronecker symbols in (29) and (31) does not vanish only if either $j_1=j_2$, $j_1'=j_2'$, or $j_1=j_2'$, $j_1'=j_2$. Since $\Sigma^{(S',S)}_{jj'jj'}(l_1,l_1',l_2,l_2')$ is independent of particular values of j and j' (see Appendix A), the sum (29) attains the form

$$\sum_{r,r'} V^{[\lambda'][\lambda]}_{r'\{n'\}r\{n\}}(l_1,l_1')V^{[\lambda'][\lambda]}_{r'\{n\}r\{n'\}}(l_2,l_2') = 2\Sigma^{(S',S)}_2(l_1,l_1',l_2,l_2')\sum_{j<j'}|\langle n'_jn'_{j'}|V|n_jn_{j'}\rangle|^2 \times \prod_{j'\neq j''\neq j}\delta_{n'_{j''},n_{j''}}$$

with

$$\Sigma^{(S',S)}_2(l_1,l_1',l_2,l_2') = \Sigma^{(S',S)}_{jj'jj'}(l_1,l_1',l_2,l_2') + \Sigma^{(S',S)}_{jj'jj'}(l_1,l_1',l_2',l_2). \tag{33}$$

Then for any two-body spin-dependent interactions $\hat{V}_a$ and $\hat{V}_b$, the sums of squared moduli of the matrix elements and their products can be written out in the form

$$\sum_{r,r'}\langle\tilde{\Psi}^{(S')}_{r'\{n'\}S'}|\hat{V}_a|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle\langle\tilde{\Psi}^{(S')}_{r'\{n'\}S'}|\hat{V}_b|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle^* = Y^{(S,2)}[\hat{V}_a,\hat{V}_b]\frac{2f_{S'}}{N(N-1)}\sum_{j<j'}|\langle n'_jn'_{j'}|V|n_jn_{j'}\rangle|^2 \times \prod_{j'\neq j''\neq j}\delta_{n'_{j''},n_{j''}} \tag{34a}$$

with $S'\leqslant S$. Each term in the sum above changes two of the spatial quantum numbers, conserving other ones. Since S and S' are equal to the spin projections, S' is unambiguously determined by the operators $\hat{V}_a$ and $\hat{V}_b$, such that $S'=S$ for $\hat{V}$, $\hat{V}_{\uparrow\uparrow}$, and $\hat{V}_{\downarrow\downarrow}$ and $S'=S+k$ for $\hat{V}^{(2)}_k$ and $\hat{V}_k$. The factors $Y^{(S,2)}[\hat{V}_a,\hat{V}_b]$ are expressed in terms of the sums $\Sigma^{(S',S)}_2(l_1,l_1',l_2,l_2')$. For example, the factor $Y^{(S,2)}[\hat{V}_{\uparrow\uparrow},\hat{V}_{\uparrow\uparrow}]$ takes the form

$$Y^{(S,2)}[\hat{V}_{\uparrow\uparrow},\hat{V}_{\uparrow\uparrow}] = 4\left[\lambda!\lambda_2!\lambda_1(\lambda_1-1)C^2_{SS}\right]^2\frac{N(N-1)}{f_S} \times \Sigma^{(S,S)}_2(\lambda_1-1,\lambda_1,\lambda_1-1,\lambda_1).$$

Similarly, the sum (31) leads to the factor

$$Y^{(S,2)}[\hat{V}_{\uparrow\uparrow},\hat{V}] = 4\lambda_1!\lambda_2!\lambda_1(\lambda_1-1)C^2_{SS}\frac{N(N-1)}{f_S} \times \left[(N-2)!+\Sigma^{(S)}_{jj'jj'}(\lambda_1-1,\lambda_1)\right].$$

The factors in the sums of squared moduli and products of matrix elements of other operators are expressed in a similar form. Explicit expressions for the factors are obtained using the normalization factors (22) and sums $\Sigma^{(S',S)}_{jj'jj'}$ and $\Sigma^{(S)}_{jj'jj'}$, calculated in Appendixes A and B, respectively. For example,

$$Y^{(S,2)}[\hat{V}_{\uparrow\uparrow},\hat{V}_{\uparrow\uparrow}] = \frac{2}{2S+3}\left[N^2(2S+1) + 2\frac{N(4S^3+8S^2+S-1)+2S(2S^3+5S^2-5)}{S+1}\right].$$

Equations (13) and (14) lead to the following factors in the sums of squared moduli of the matrix elements of spherical tensor components and their products:

$$Y^{(S,2)}\left[\hat{V}^{(2)}_0,\hat{V}^{(2)}_0\right] = \frac{S(2S-1)}{6(2S+3)}\left(3\frac{(N+2)^2}{S+1}-4S\right), \tag{34b}$$

$$Y^{(S,2)}[\hat{V}_0,\hat{V}_0] = S\left(4S+\frac{N^2-4}{S+1}\right), \tag{34c}$$

$$Y^{(S,2)}\left[\hat{V}^{(2)}_0,\hat{V}_0\right] = \sqrt{\frac{2}{3}}\frac{(N+2)S(2S-1)}{S+1}, \tag{34d}$$

$$Y^{(S,2)}\left[\hat{V}^{(2)}_0,\hat{V}\right] = 4\sqrt{\frac{2}{3}}S(2S-1), \tag{34e}$$

$$Y^{(S,2)}[\hat{V}_0,\hat{V}] = 8S(N-1), \tag{34f}$$

$$Y^{(S,2)}\left[\hat{V}^{(2)}_{-1},\hat{V}^{(2)}_{-1}\right] = \frac{(N+2)(N-2S+2)(S-1)}{2(S+1)}, \tag{34g}$$

$$Y^{(S,2)}[\hat{V}_{-1},\hat{V}_{-1}] = (N-2)(N-2S+2), \tag{34h}$$

$$Y^{(S,2)}\left[\hat{V}^{(2)}_{-1},\hat{V}_{-1}\right] = \sqrt{2}(N-2S+2)(S-1), \tag{34i}$$

$$Y^{(S,2)}\left[\hat{V}^{(2)}_{-2},\hat{V}^{(2)}_{-2}\right] = \frac{1}{2}(N-2S+2)(N-2S+4). \tag{34j}$$

The sum of squared moduli of the matrix elements of the spin-independent interactions (I.47a) can be expressed in the case of bosons with the zero-range potentials (11) in the form (39a) too with

$$Y^{(S,2)}[\hat{V},\hat{V}] = 6N(N-2)+8S(S+1). \tag{34k}$$

The case of a single changed quantum number will be considered elsewhere.

E. Conserving set of spatial quantum numbers

If the set of spatial quantum numbers is unchanged, $\{n\}=\{n'\}$, the Kronecker symbols in sums (29) and (31) are equal to 1 for any j_1, j_2, j_1', and j_2'. Then these sums contain

$$\begin{aligned}\sum_{j_1\neq j_1'}\sum_{j_2\neq j_2'}\Sigma_{j_1j_1'j_2j_2'}V_{j_1j_1'}V_{j_2j_2'}&=\Sigma_4\Bigg(\sum_{j\neq j'}V_{jj'}\Bigg)^2+(\Sigma_3-4\Sigma_4)\sum_{j'\neq j\neq j''}V_{jj'}V_{jj''}\\&\quad+(\Sigma_2-\Sigma_3+2\Sigma_4)\sum_{j\neq j'}V_{jj'}^2,\end{aligned}\tag{35}$$

where the matrix elements of zero-range interactions (11) are symmetric over permutations of n_j and $n_{j'}$,

$$\begin{aligned}V_{jj'}&=\langle n_jn_{j'}|V|n_jn_{j'}\rangle=\langle n_{j'}n_j|V|n_jn_{j'}\rangle=\langle n_jn_{j'}|V|n_{j'}n_j\rangle\\&=\int d^Dr|\varphi_{n_j}(\mathbf{r})\varphi_{n_{j'}}(\mathbf{r})|^2,\end{aligned}\tag{36}$$

and $\Sigma_{j_1j_1'j_2j_2'}$ can be either $\Sigma^{(S',S)}_{j_1j_1'j_2j_2'}(l_1,l_1',l_2,l_2')$ or $\Sigma^{(S)}_{j_1j_1'j_2j_2'}(l,l')$ [see Eqs. (30) and (32)] with arbitrary superscripts and arguments. These functions depend on relations between their subscripts, rather than the subscript specific values (see Appendixes A and B). Then $\Sigma_4=\Sigma_{j_1j_1'j_2j_2'}$ for $j_1\neq j_2\neq j_1'$ and $j_1\neq j_2'\neq j_1'$, $\Sigma_3=\Sigma_{jj'jj''}+\Sigma_{jj'j''j}+\Sigma_{j'jjj''}+\Sigma_{j'jj''j}$ for $j'\neq j\neq j''\neq j'$, and $\Sigma_2=\Sigma_{jj'jj'}+\Sigma_{jj'j'j}$ for $j\neq j'$. The sum (35) can be further transformed to

$$\begin{aligned}\sum_{j_1\neq j_1'}\sum_{j_2\neq j_2'}\Sigma_{j_1j_1'j_2j_2'}V_{j_1j_1'}V_{j_2j_2'}&=N(N-1)[(N-2)(N-3)\Sigma_4+(N-2)\Sigma_3+\Sigma_2]\langle V\rangle^2\\&\quad+N(N-1)^2(\Sigma_3-4\Sigma_4)\langle\Delta_1V\rangle^2\\&\quad+N(N-1)(\Sigma_2-\Sigma_3+2\Sigma_4)(\langle\Delta_2V\rangle^2.\end{aligned}$$

Here

$$\langle V\rangle=\frac{2}{N(N-1)}\sum_{j<j'}V_{jj'}\tag{37}$$

is the average value of the matrix elements (36) and

$$\begin{aligned}\langle\Delta_1V\rangle^2&=\frac{1}{N}\sum_{j=1}^{N}\Bigg(\frac{1}{N-1}\sum_{j'\neq j}V_{jj'}-\langle V\rangle\Bigg)^2\\\langle\Delta_2V\rangle^2&=\frac{2}{N(N-1)}\sum_{j<j'}(V_{jj'}-\langle V\rangle)^2\end{aligned}\tag{38}$$

measure their average deviations [in consistency with (I.48)]. Then the sums of squared moduli of the matrix elements and their products can be written out in the form

$$\begin{aligned}&\sum_{r,r'}\langle\tilde\Psi^{(S')}_{r'\{n\}S'}|\hat V_a|\tilde\Psi^{(S)}_{r\{n\}S}\rangle\langle\tilde\Psi^{(S')}_{r'\{n\}S'}|\hat V_b|\tilde\Psi^{(S)}_{r\{n\}S}\rangle^*\\&=f_{S'}\big(Y_0^{(S,0)}[\hat V_a,\hat V_b]\langle V\rangle^2+Y_1^{(S,0)}[\hat V_a,\hat V_b]\langle\Delta_1V\rangle^2\\&\quad+Y_2^{(S,0)}[\hat V_a,\hat V_b]\langle\Delta_2V\rangle^2\big)\end{aligned}\tag{39a}$$

with $S'\leqslant S$. The factors $Y_i^{(S,0)}$ here are calculated using results of Appendixes A, B, and C. The first factor can be represented for all considered $\hat V_a$ and $\hat V_b$ as

$$Y_0^{(S,0)}[\hat V_a,\hat V_b]=\delta_{SS'}Y^{(S)}[\hat V_a]Y^{(S)}[\hat V_b]\tag{39b}$$

[see Eq. (28)]. Since $S'-S$ is unambiguously determined by $\hat V_a$ and $\hat V_b$ ($S'=S$ for $\hat V$ and $S'=S+k$ for $\hat V_k^{(2)}$ and $\hat V_k$), $Y_0^{(S,0)}[\hat V_a,\hat V_b]=0$ for $k\neq0$ components of the spherical vectors and tensors, when $S\neq S'$. Other factors are expressed as

$$Y_1^{(S,0)}\big[\hat V_0^{(2)},\hat V_0^{(2)}\big]=-\frac{(N-1)(N-2S)(N+2S+2)S(2S-1)}{3(N-2)(N-3)(2S+3)}\left(3\frac{N+3}{S+1}-8S\right),\tag{39c}$$

$$Y_2^{(S,0)}\big[\hat V_0^{(2)},\hat V_0^{(2)}\big]=\frac{(N-2S)(N+2S+2)S(2S-1)}{6(N-2)(N-3)(2S+3)}\left(3N\frac{N-1}{S+1}-8S\right),\tag{39d}$$

$$Y_1^{(S,0)}[\hat V_0,\hat V_0]=\frac{(N-1)(N-2S)(N+2S+2)S}{S+1},\tag{39e}$$

$$Y_1^{(S,0)}\big[\hat V_0^{(2)},\hat V_0\big]=\sqrt{\frac{2}{3}}\frac{(N-1)(N-2S)(N+2S+2)S(2S-1)}{(N-2)(S+1)},\tag{39f}$$

$$Y_1^{(S,0)}\big[\hat V_0^{(2)},\hat V\big]=2\sqrt{\frac{2}{3}}\frac{(N-1)(N-2S)(N+2S+2)S(2S-1)}{(N-2)(N-3)},\tag{39g}$$

$$Y_2^{(S,0)}\big[\hat V_0^{(2)},\hat V\big]=-\sqrt{\frac{2}{3}}\frac{(N-2S)(N+2S+2)S(2S-1)}{(N-2)(N-3)},\tag{39h}$$

$$Y_1^{(S,0)}[\hat V_0,\hat V]=2\frac{(N-1)(N-2S)(N+2S+2)S}{N-2},\tag{39i}$$

$$Y_1^{(S,0)}\big[\hat V_{-1}^{(2)},\hat V_{-1}^{(2)}\big]=(N-1)(N-2S+2)(S-1)\frac{2(N+1)S^2-N(N+3)}{(N-2)(N-3)(S+1)},\tag{39j}$$

$$Y_2^{(S,0)}\big[\hat V_{-1}^{(2)},\hat V_{-1}^{(2)}\big]=\frac{(N-1)(N-2S)(N+2S)(N-2S+2)(S-1)}{2(N-2)(N-3)(S+1)},\tag{39k}$$

$$Y_1^{(S,0)}[\hat{V}_{-1},\hat{V}_{-1}] = N(N-1)(N-2S+2), \tag{39l}$$

$$Y_1^{(S,0)}\big[\hat{V}_{-1}^{(2)},\hat{V}_{-1}\big] = \frac{\sqrt{2}N(N-1)(N-2S+2)(S-1)}{(N-2)}, \tag{39m}$$

$$Y_1^{(S,0)}\big[\hat{V}_{-2}^{(2)},\hat{V}_{-2}^{(2)}\big] = -\frac{(N-1)^2(N-2S+2)(N-2S+4)}{(N-2)(N-3)}, \tag{39n}$$

$$Y_2^{(S,0)}\big[\hat{V}_{-2}^{(2)},\hat{V}_{-2}^{(2)}\big] = \frac{(N-1)(N-2S+2)(N-2S+4)}{2(N-3)}. \tag{39o}$$

The vanishing factors are omitted above, namely $Y_2^{(S,0)}[\hat{V}_a,\hat{V}_b] = 0$ when $\hat{V}_a$ or $\hat{V}_b$ is $\hat{V}_k$. The sum of squared moduli of the matrix elements of the spin-independent interactions (I.47b) can be expressed for bosons and the zero-range potentials (11) in the form (39a) too with

$$Y_1^{(S,0)}[\hat{V},\hat{V}] = -\frac{(N-1)(N-2S)(N+2S+2)}{(N-3)} \times\left(3-4S\frac{S+1}{N-2}\right), \tag{39p}$$

$$Y_2^{(S,0)}[\hat{V},\hat{V}] = (N-2S)(N+2S+2) \times\frac{3N(N-4)-4S(S+1)+12}{2(N-2)(N-3)}. \tag{39q}$$

They are equal to the factors (I.47c).

Thus, sums of matrix elements and their squared moduli are expressed in terms of universal factors, which are independent of the spatial orbitals, and sums of one-body matrix elements (or their squared moduli), which are independent of many-body spins and the spin dependence of the interaction. The sum rules, combined with the spin-projection dependencies (9) and (10), provide information on each matrix element for any two-body spin-dependent interaction between the particles.

IV. MULTIPLET ENERGIES AND CORRELATIONS FOR WEAKLY INTERACTING GASES

A. Average multiplet energies and energy widths

Consider a general spin-dependent two-body interaction, conserving the particle spins,

$$\hat{V}_{\rm tot} = \tfrac{1}{2}g_{\uparrow\uparrow}\hat{V}_{\uparrow\uparrow} + \tfrac{1}{2}g_{\downarrow\downarrow}\hat{V}_{\downarrow\downarrow} + g_{\uparrow\downarrow}\hat{V}_{\uparrow\downarrow}, \tag{40}$$

where the potentials are defined by Eqs. (4a)–(4c) with the zero-range potential function (11). Here the interaction strengths $g_{\sigma\sigma'}$ are proportional to the s-wave elastic scattering lengthes $a_{\sigma\sigma'}$ for corresponding pairs of spin states. For example, in three-dimensional geometry $g_{\sigma\sigma'} = 4\pi\hbar^2 a_{\sigma\sigma'}/m$, where m is the particle's mass. The factors $\frac{1}{2}$ in Eq. (40) appears due to double counting of the interacting pairs in $\hat{V}_{\uparrow\uparrow}$ (4a) and $\hat{V}_{\downarrow\downarrow}$ (4b).

In the case of weak interaction, the average multiplet energy can be evaluated in the zero order of the degenerate perturbation theory, in the same way as in the case of spin-independent interactions [see derivation of Eq. (I.52)]

$$\bar{E}_{SS_z} = \frac{1}{f_S}\sum_r \big\langle \tilde{\Psi}^{(S)}_{r\{n\}S_z}\big|\hat{V}_{\rm tot}\big|\tilde{\Psi}^{(S)}_{r\{n\}S_z}\big\rangle \tag{41}$$

(in the case of spin-dependent interactions the energies depend on the total spin projection S_z).

For bosons with zero-range interactions, matrix elements of the potentials are related to ones of the irreducible spherical tensor components by Eqs. (4a)–(4c) and (13),

$$\langle\Psi'|\hat{V}_{\uparrow\uparrow}|\Psi\rangle = \langle\Psi'|\sqrt{\frac{2}{3}}\hat{V}_0^{(2)} + \hat{V}_0 + \frac{1}{3}\hat{V}|\Psi\rangle,$$

$$\langle\Psi'|\hat{V}_{\downarrow\downarrow}|\Psi\rangle = \langle\Psi'|\sqrt{\frac{2}{3}}\hat{V}_0^{(2)} - \hat{V}_0 + \frac{1}{3}\hat{V}|\Psi\rangle,$$

$$\langle\Psi'|\hat{V}_{\uparrow\downarrow}|\Psi\rangle = \langle\Psi'| -\sqrt{\frac{2}{3}}\hat{V}_0^{(2)} + \frac{1}{6}\hat{V}|\Psi\rangle.$$

These equations allow us to expand the interaction $\hat{V}_{\rm tot}$ in terms of irreducible spherical tensors, which matrix elements can be related to the ones for the maximal allowed spin projections by Eqs. (9) and (10). Then the sum rules (28) lead to

$$\bar{E}_{SS_z} = \frac{1}{2}\bigg(gY^{(S)}[\hat{V}] + g_- X^{(S,S,1)}_{S_z0}Y^{(S)}[\hat{V}_0] + \sqrt{\frac{2}{3}}g_+X^{(S,S,2)}_{S_z0}Y^{(S)}\big[\hat{V}_0^{(2)}\big]\bigg)\langle V\rangle,$$

where $g = (g_{\uparrow\uparrow} + g_{\downarrow\downarrow} + g_{\uparrow\downarrow})/3$, $g_+ = g_{\uparrow\uparrow} + g_{\downarrow\downarrow} - 2g_{\uparrow\downarrow}$, $g_- = g_{\uparrow\uparrow} - g_{\downarrow\downarrow}$, and the average matrix element $\langle V\rangle$ is defined by Eq. (37). Substituting the coefficients X and Y from Table I in [1], Table I, and Eq. (28) one gets

$$\bar{E}_{SS_z} = g\bigg[\frac{3}{4}N(N-2) + S(S+1) - \frac{1}{3}S(S+1)\frac{g_+}{g} + S_z(N-1)\frac{g_-}{g} + S_z^2\frac{g_+}{g}\bigg]\langle V\rangle. \tag{42}$$

Here the first two terms in the square brackets provide the average multiplet energy (I.52) for spin-independent interactions. Spin dependence of the interactions leads to the third term, which is independent of the total spin projection S_z, as well as to the linear and quadratic in S_z shifts (the fourth and fifth terms, respectively). The corrections are proportional to the ratios $g_\pm/g$, which are determined by the scattering lengths. For example, $g_+/g \approx -0.001$ and $g_-/g \approx -0.049$ for ^{87}Rb. In this case, the two states, generally used in experiments, $|\uparrow\rangle = |F=2,m_f=-1\rangle$ and $|\downarrow\rangle = |F=1,m_f=1\rangle$, have the scattering lengths [37] $a_{\uparrow\uparrow} \approx 95.5a_B$, $a_{\downarrow\downarrow} \approx 100.4a_B$, and $a_{\uparrow\downarrow} \approx 98.0a_B$, where a_B is the Bohr radius. One-body spin-dependent interactions with external fields lead only to linear shifts [see Eq. (I.54)].

The root-mean-square multiplet width can be evaluated in the same way as in the case of spin-independent interactions [see derivation of Eq. (I.53)]

$$\langle\Delta E_{SS_z}\rangle^2=\frac{1}{f_S}\sum_{r,r'}\left|\left\langle\tilde{\Psi}^{(S)}_{r'\{n\}S_z}\middle|\hat{V}_{\rm tot}\middle|\tilde{\Psi}^{(S)}_{r\{n\}S_z}\right\rangle\right|^2-\bar{E}^2_{SS_z}.$$

Expanding the interaction $\hat{V}_{\rm tot}$ in terms of irreducible spherical tensors, expressing their matrix elements in terms of the ones for the maximal allowed spin projections, and applying the sum rules (39) we get

$$\begin{aligned}\langle\Delta E_{SS_z}\rangle^2=&\frac{1}{4}\sum_{i=1}^{2}\Big[g^2Y_i^{(S,0)}[\hat{V},\hat{V}]+\big(g_-X^{(S,S,1)}_{S_z0}\big)^2Y_i^{(S,0)}[\hat{V}_0,\hat{V}_0]\\&+\frac{2}{3}\big(g_+X^{(S,S,2)}_{S_z0}\big)^2Y_i^{(S,0)}\big[\hat{V}_0^{(2)},\hat{V}_0^{(2)}\big]\\&+2g_-gX^{(S,S,1)}_{S_z0}Y_i^{(S,0)}[\hat{V}_0,\hat{V}]+2\sqrt{\frac{2}{3}}g_+gX^{(S,S,2)}_{S_z0}\\&\times Y_i^{(S,0)}\big[\hat{V}_0^{(2)},\hat{V}\big]+2\sqrt{\frac{2}{3}}g_+g_-X^{(S,S,1)}_{S_z0}X^{(S,S,2)}_{S_z0}\\&\times Y_i^{(S,0)}\big[\hat{V}_0^{(2)},\hat{V}_0\big]\Big]\langle\Delta_iV\rangle^2.\end{aligned}$$

Here the matrix element deviations $\langle\Delta_iV\rangle^2$ are defined by Eq. (38) and the terms proportional to $\langle V\rangle^2$ are canceled due to relation (39b). The first term in the square brackets gives the width for the spin-independent interactions (I.53). Corrections due to spin dependence of the interactions are proportional to the small parameters $g_\pm/g$. Leading terms in the coefficients before each power of S_z can be obtained using explicit expressions for X from Table I in [1] and Table I,

$$\begin{aligned}\langle\Delta E_{SS_z}\rangle^2=&\frac{g^2}{4}\sum_{i=1}^{2}\Big[Y_i^{(S,0)}[\hat{V},\hat{V}]-2\sqrt{\frac{2}{3}}\frac{S+1}{2S-1}\\&\times Y_i^{(S,0)}\big[\hat{V}_0^{(2)},\hat{V}\big]\frac{g_+}{g}+\frac{2}{S}Y_i^{(S,0)}[\hat{V}_0,\hat{V}]\frac{g_-}{g}S_z\\&+\frac{2\sqrt{6}}{S(2S-1)}Y_i^{(S,0)}\big[\hat{V}_0^{(2)},\hat{V}\big]\frac{g_+}{g}S_z^2+\frac{2\sqrt{6}}{S^2(2S-1)}\\&\times Y_i^{(S,0)}\big[\hat{V}_0^{(2)},\hat{V}_0\big]\frac{g_-g_+}{g^2}S_z^3+\frac{6}{S^2(2S-1)^2}\\&\times Y_i^{(S,0)}\big[\hat{V}_0^{(2)},\hat{V}_0^{(2)}\big]\frac{g_+^2}{g^2}S_z^4\Big]\langle\Delta_iV\rangle^2.\end{aligned}\quad(43)$$

The consideration above was devoted to the case of bosons. For fermions, matrix elements of $\hat{V}_{\uparrow\uparrow}$, and $\hat{V}_{\downarrow\downarrow}$ vanish, according to the Pauli principle (see Sec. III A). Then, due to Eqs. (4c) and (15) matrix elements of $\hat{V}_{\rm tot}$ are equal to ones of $g_{\uparrow\downarrow}\hat{V}$. Therefore, the muliplet average energies and energy widths are independent of S_z and can be calculated using Eqs. (I.52) and (I.53) for spin-independent interactions.

B. Average correlations

The probabilities of finding two particles with given (either equal or different) spins in the same point, the two-body local spin-dependent correlations are expectation values of operators

$$\hat{\rho}_{\sigma_1\sigma_2}=\delta(\mathbf{r}_1-\mathbf{r}_2)|\sigma_1(1)\rangle|\sigma_2(2)\rangle\langle\sigma_1(1)|\langle\sigma_2(2)|.\quad(44)$$

The spin projection σ_j can be either $\uparrow$ or $\downarrow$. Due to permutation symmetry of the total wave functions, the expectation values of $\hat{\rho}_{\sigma_1\sigma_2}$ are proportional to matrix elements of the spin-dependent potentials $\hat{V}_{\sigma_1\sigma_2}$ with the potential function (11). The multiplet-averaged correlations can be evaluated in the same way as the average multiplet energy (41). However, Eq. (41) already contains all necessary information, as, according to the Hellmann-Feinman theorem [38,39], the correlations are proportional to derivatives of the average energy over respective coupling constants

$$\begin{aligned}\bar{\rho}^{(S,S_z)}_{\sigma_1\sigma_2}&=\frac{1}{f_S}\sum_r\left\langle\tilde{\Psi}^{(S)}_{r\{n\}S_z}\middle|\hat{\rho}_{\sigma_1\sigma_2}\middle|\tilde{\Psi}^{(S)}_{r\{n\}S_z}\right\rangle\\&=\frac{1+\delta_{\sigma_1\sigma_2}}{N(N-1)}\frac{\partial}{\partial g_{\sigma_1\sigma_2}}\bar{E}_{SS_z}.\end{aligned}$$

Then the dependence of the multiplet-averaged correlations

$$\begin{aligned}\bar{\rho}^{(S,S_z)}_{\uparrow\uparrow}=&\Big(\frac{1}{3}Y^{(S)}[\hat{V}]+X^{(S,S,1)}_{S_z0}Y^{(S)}[\hat{V}_0]\\&+\sqrt{\frac{2}{3}}X^{(S,S,2)}_{S_z0}Y^{(S)}\big[\hat{V}_0^{(2)}\big]\Big)\frac{1}{N(N-1)}\langle\rho_2(0)\rangle,\\\bar{\rho}^{(S,S_z)}_{\downarrow\downarrow}=&\Big(\frac{1}{3}Y^{(S)}[\hat{V}]-X^{(S,S,1)}_{S_z0}Y^{(S)}[\hat{V}_0]\\&+\sqrt{\frac{2}{3}}X^{(S,S,2)}_{S_z0}Y^{(S)}\big[\hat{V}_0^{(2)}\big]\Big)\frac{1}{N(N-1)}\langle\rho_2(0)\rangle,\\\bar{\rho}^{(S,S_z)}_{\uparrow\downarrow}=&\Big(\frac{1}{6}Y^{(S)}[\hat{V}]-\sqrt{\frac{2}{3}}X^{(S,S,2)}_{S_z0}Y^{(S)}\big[\hat{V}_0^{(2)}\big]\Big)\\&\times\frac{1}{N(N-1)}\langle\rho_2(0)\rangle\end{aligned}$$

on the total many-body spin S and its projection S_z is factorized to the universal factors, which are independent of the spatial Hamiltonian and occupied spatial orbitals. These factors are expressed in terms of the coefficients X and Y. The dependence on the spatial state is given by the average two-body density [19], $\langle\rho_2(0)\rangle$, which is independent of S and S_z and equal to the average matrix element $\langle V\rangle$ (37) for the potential function (11), $\langle\rho_2(0)\rangle=\langle V\rangle$. Similar factorization was proved [19] for spin-independent local correlations of particles with arbitrary spins. Substitution the coefficients X and Y from Table I in [1], Table I, and Eq. (28) leads to explicit expressions for the universal factors in terms of S and S_z,

$$\begin{aligned}\bar{\rho}^{(S,S_z)}_{\uparrow\uparrow}&=\frac{\langle\rho_2(0)\rangle}{N(N-1)}\Big(\frac{1}{2}N(N-2)+2(N-1)S_z+2S_z^2\Big),\\\bar{\rho}^{(S,S_z)}_{\downarrow\downarrow}&=\frac{\langle\rho_2(0)\rangle}{N(N-1)}\Big(\frac{1}{2}N(N-2)-2(N-1)S_z+2S_z^2\Big),\\\bar{\rho}^{(S,S_z)}_{\uparrow\downarrow}&=\frac{\langle\rho_2(0)\rangle}{N(N-1)}\Big(\frac{1}{4}N(N-2)+S(S+1)-2S_z^2\Big).\end{aligned}\quad(45)$$

The local spin-independent correlations [19] are multiplet-averaged expectation values of $\delta(\mathbf{r}_1-\mathbf{r}_2)$ and can be calculated with the characters from Table II in [1] for both bosons and fermions (the signs + and −, respectively, below),

$$\bar{\rho}_2^{[\lambda]}(0) = \left(1 \pm \frac{\chi_S(\{2\})}{f_S}\right)\langle\rho_2(0)\rangle = \left(1 \pm \frac{4S^2 + N^2 + 4S - 4N}{2N(N-1)}\right)\langle\rho_2(0)\rangle. \quad (46)$$

They are related to spin-dependent correlations, $\bar{\rho}_2^{[\lambda]}(0) = \bar{\rho}_{\uparrow\uparrow}^{(S,S_z)} + \bar{\rho}_{\downarrow\downarrow}^{(S,S_z)} + 2\bar{\rho}_{\uparrow\downarrow}^{(S,S_z)}$, as can be proved in the same way as (12), and are independent of S_z.

In an alternative description, each particle is characterized by its spin projection and coordinate, and the total wave function is symmetrized for bosons or antisymmetrized for fermions over permutations of all particles [see Eq. (I.19)],

$$\tilde{\Psi}_{\{n\}\{\sigma\}} = (N!)^{-1/2} \sum_{\mathcal{P}} \text{sgn}(\mathcal{P}) \prod_{j=1}^{N} \varphi_{n_{\mathcal{P}j}}(\mathbf{r}_j)|\sigma_{\mathcal{P}j}(j)\rangle, \quad (47)$$

where the factor sgn($\mathcal{P}$) is the permutation parity for fermions and sgn($\mathcal{P}$) ≡ 1 for bosons. Given total spin projection S_z, the set $\{\sigma\}$ contains $N_\uparrow = N/2 + S_z$ spins ↑ and $N_\downarrow = N/2 - S_z$ spins ↓. For these wave functions the correlations are calculated as expectation values of the operators (44) and averaged over all distinct choices of $N_\uparrow$ particles with spin up, leading to

$$\bar{\rho}_{\uparrow\uparrow}^{(N_\uparrow,N_\downarrow)} = \frac{1 + \text{sgn}(\mathcal{P}_{12})}{N(N-1)} N_\uparrow(N_\uparrow - 1)\langle\rho_2(0)\rangle,$$
$$\bar{\rho}_{\downarrow\downarrow}^{(N_\uparrow,N_\downarrow)} = \frac{1 + \text{sgn}(\mathcal{P}_{12})}{N(N-1)} N_\downarrow(N_\downarrow - 1)\langle\rho_2(0)\rangle,$$
$$\bar{\rho}_{\uparrow\downarrow}^{(N_\uparrow,N_\downarrow)} = \frac{\langle\rho_2(0)\rangle}{N(N-1)} N_\uparrow N_\downarrow.$$

The transposition parity sgn($\mathcal{P}_{12}$) = 1 leads to the factor 2 in $\bar{\rho}_{\uparrow\uparrow}^{(N_\uparrow,N_\downarrow)}$ and $\bar{\rho}_{\uparrow\uparrow}^{(N_\uparrow,N_\downarrow)}$ for bosons. For fermions, sgn($\mathcal{P}_{12}$) = −1 and correlations of particles with the same spins vanish, according to the Pauli exclusion principle. Using relations between S_z and $N_{\uparrow\downarrow}$, one can see that the average correlations of bosons with the same spins are the same as for wave functions with defined collective spins and individual spin projections, $\bar{\rho}_{\uparrow\uparrow}^{(S,S_z)} = \bar{\rho}_{\uparrow\uparrow}^{(N_\uparrow,N_\downarrow)}$, $\bar{\rho}_{\downarrow\downarrow}^{(S,S_z)} = \bar{\rho}_{\uparrow\uparrow}^{(N_\uparrow,N_\downarrow)}$. However, average correlations of particles with opposite spins are different,

$$\bar{\rho}_{\uparrow\downarrow}^{(S,S_z)} = \bar{\rho}_{\uparrow\downarrow}^{(N_\uparrow,N_\downarrow)} + \frac{\langle\rho_2(0)\rangle}{N(N-1)}\left(S^2 - S_z^2 + S - \frac{N}{2}\right).$$

The same is valid for average local spin-independent correlations, calculated as a sum of spin-dependent correlations. For the defined individual spin projections we have for both bosons and fermions (the signs + and −, respectively, below)

$$\bar{\rho}_{\uparrow\uparrow}^{(N_\uparrow,N_\downarrow)} + \bar{\rho}_{\downarrow\downarrow}^{(N_\uparrow,N_\downarrow)} + 2\bar{\rho}_{\uparrow\downarrow}^{(N_\uparrow,N_\downarrow)} = \left(1 \pm \frac{N^2 + 4S_z^2 - 2N}{2N(N-1)}\right)\langle\rho_2(0)\rangle,$$

which depends on the total spin projection, unlike $\bar{\rho}_2^{[\lambda]}(0)$ [see Eq. (46)]. For fermions, the average correlations of particles with opposite spins, being equal to a half spin-independent one, are different for the two kinds of states too. Thus the spin-independent correlations, as well as the correlations of particles with opposite spins, allow us to determine the kind of the many-body state.

V. CONCLUSIONS

Matrix elements of spin-dependent two-body interactions [Eqs. (4), (6), and (7)] in the basis with collective spin and spatial wave functions (16) can be calculated with group-theoretical methods. These matrix elements agree to the selection rules [19]. The interactions can be decomposed into irreducible spherical tensors, whose explicit dependencies on the total spin projection [Eqs. (9) and (10)] are obtained using the Wigner-Eckart theorem. Analytic expressions are derived for sums of these matrix elements (28) and their squared moduli [Eqs. (34) and (39)] over wave functions with the fixed total spin, its projection, and the set of spatial orbitals. Dependence on the many-body states in these sums is given by the $3j$ Wigner symbols and the universal factors $Y^{(S)}$, $Y^{(S,2)}$, $Y_0^{(S,0)}$, $Y_1^{(S,0)}$, and $Y_2^{(S,0)}$. These factors are independent of details of one-body Hamiltonians and are expressed in terms of the total spin and number of particles. The sum rules can be applied to the evaluation of changes of the spin-multiplet average energies (42) and energy widths (43) due to weak spin-dependent interactions. Mutiplet-averaged two-body spin-dependent correlations (45), calculated with the sum rules, are factorized to universal factors, which are independent of the spatial orbitals, and the average density, which is independent of many-body spins. The difference between these correlations and ones for the many-body states with defined individual spin projections allows identification of the many-body state kind. Other possible applications of the sum rules include estimates of the spin-multiplet depletion rates due to spin-dependent two-body perturbations.

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APPENDIX A: CALCULATION OF THE SUMS (30)

The sums (30) and (32) contain the Young orthogonal matrix elements $D_{[0][0]}^{[\lambda]}(\mathcal{R})$, which have been calculated by Goddard [40] in the following way. Each permutation $\mathcal{R}$ can be represented as

$$\mathcal{R} = \prod_{k=1}^{n_{\text{ex}}} \mathcal{P}_{i'_k i''_k} \mathcal{P}' \mathcal{P}'', \quad \text{(A1)}$$

where $\mathcal{P}'$ are permutations of symbols in the first row of the Young tableau [0] (λ_1 first symbols), $\mathcal{P}''$ are permutations of symbols in the second row (λ_2 last symbols), and $\mathcal{P}_{i'_k i''_k}$ transpose symbols between the rows as $i'_k \leqslant \lambda_1$ and $i''_k > \lambda_1$. Then [40] the matrix element is inversely proportional to the binomial coefficient,

$$D_{[0][0]}^{[\lambda]}(\mathcal{R}) = (-1)^{n_{\rm ex}} \binom{\lambda_1}{n_{\rm ex}}^{-1} = (-1)^{n_{\rm ex}} \frac{n_{\rm ex}!(\lambda_1 - n_{\rm ex})!}{\lambda_1!}. \tag{A2}$$

Using relations (23) and (18) and substitution $\mathcal{R} = \mathcal{Q}\mathcal{P}^{-1}$, the sum (30) can be represented in the following form:

$$\Sigma_{j_1 j_1' j_2 j_2'}^{(S',S)}(l_1,l_1',l_2,l_2') = \sum_{\mathcal{R}} D_{[0][0]}^{[\lambda']}(\mathcal{R}) D_{[0][0]}^{[\lambda]}(\mathcal{R}) \sum_{\mathcal{P}} \delta_{l_1,\mathcal{P}j_1} \delta_{l_1',\mathcal{P}j_1'} \delta_{l_2,\mathcal{R}\mathcal{P}j_2} \delta_{l_2',\mathcal{R}\mathcal{P}j_2'},$$

where $\lambda = [N/2 + S, N/2 - S]$ and $\lambda' = [N/2 + S', N/2 - S']$. Only the sums with $j_1 \neq j_1'$ and $j_2 \neq j_2'$ are used here. This implies $l_1 \neq l_1'$ and $l_2 \neq l_2'$. The sum remains unchanged on simultaneous permutation of arguments and corresponding subscripts, $\Sigma_{j_1 j_1' j_2 j_2'}^{(S',S)}(l_1,l_1',l_2,l_2') = \Sigma_{j_1' j_1 j_2 j_2'}^{(S',S)}(l_1',l_1,l_2,l_2') = \Sigma_{j_1 j_1' j_2' j_2}^{(S',S)}(l_1,l_1',l_2',l_2)$.

If $j_1 = j_2$ and $j_1' = j_2'$,

$$\Sigma_{jj'jj'}^{(S',S)}(l_1,l_1',l_2,l_2') = (N-2)! \sum_{\mathcal{R}} D_{[0][0]}^{[\lambda']}(\mathcal{R}) D_{[0][0]}^{[\lambda]}(\mathcal{R}) \delta_{l_2,\mathcal{R}l_1} \delta_{l_2',\mathcal{R}l_1'}, \tag{A3}$$

since there are $(N-2)!$ permutations $\mathcal{P}$ such that $l_1 = \mathcal{P}j_1$ and $l_1' = \mathcal{P}j_1'$. This sum is independent of j and j'. Due to the invariance mentioned above, $\Sigma_{jj'j'j}^{(S',S)}(l_1,l_1',l_2,l_2') = \Sigma_{jj'jj'}^{(S',S)}(l_1,l_1',l_2',l_2)$ and $\Sigma_{jj'jj'}^{(S',S)}(l_1',l_1,l_2',l_2) = \Sigma_{jj'jj'}^{(S',S)}(l_1,l_1',l_2,l_2')$. The identity $\Sigma_{jj'jj'}^{(S,S')}(l_1,l_1',l_2,l_2') = \Sigma_{jj'jj'}^{(S,S')}(l_2,l_2',l_1,l_1')$ can be proved by the substitution $\mathcal{R} = \mathcal{R}^{-1}$.

If $j_1' = j_2'$, but $j_1 \neq j_2$, we have

$$\sum_{\mathcal{P}} \delta_{l_1,\mathcal{P}j_1} \delta_{l_1',\mathcal{P}j'} \delta_{l_2,\mathcal{R}\mathcal{P}j_2} \delta_{l_2',\mathcal{R}\mathcal{P}j'} = \delta_{l_2',\mathcal{R}l_1'} \sum_{l_1 \neq l \neq l_1'} \delta_{l_2,\mathcal{R}l} \sum_{\mathcal{P}} \delta_{l_1,\mathcal{P}j_1} \delta_{l,\mathcal{P}j_2} \delta_{l_1',\mathcal{P}j'} = (N-3)! \delta_{l_2',\mathcal{R}l_1'} \sum_{l} \delta_{l_2,\mathcal{R}l}(1 - \delta_{ll_1} - \delta_{ll_1'}).$$

Then

$$\begin{aligned}\Sigma_{j_1 j' j_2 j'}^{(S',S)}(l_1,l_1',l_2,l_2') &= \sum_{\mathcal{R}} D_{[0][0]}^{[\lambda']}(\mathcal{R}) D_{[0][0]}^{[\lambda]}(\mathcal{R})(N-3)! \delta_{l_2',\mathcal{R}l_1'} \left(1 - \delta_{l_2,\mathcal{R}l_1} - \delta_{l_2,\mathcal{R}l_1'}\right) \\ &= \frac{1}{(N-1)(N-2)} \Sigma_{jj}^{(S',S)}(l_1',l_2') - \frac{1}{N-2} \Sigma_{jj'jj'}^{(S',S)}(l_1,l_1',l_2,l_2')\end{aligned}$$

($\delta_{l_2',\mathcal{R}l_1'} \delta_{l_2,\mathcal{R}l_1'} = 0$, since $l_2 \neq l_2'$) is independent of j' and $j_1 \neq j_2$. Here the sum

$$\Sigma_{jj}^{(S',S)}(l,l') = (N-1)! \sum_{\mathcal{R}} D_{[0][0]}^{[\lambda']}(\mathcal{R}) D_{[0][0]}^{[\lambda]}(\mathcal{R}) \delta_{l',\mathcal{R}l} \tag{A4}$$

is calculated in Appendix C. The sum

$$\Sigma_3^{(S',S)}(l_1,l_1',l_2,l_2') = \Sigma_{j'j_1j'j_2}^{(S',S)}(l_1,l_1',l_2,l_2') + \Sigma_{j'j_1j_2j'}^{(S',S)}(l_1,l_1',l_2,l_2') + \Sigma_{j_1j'j'j_2}^{(S',S)}(l_1,l_1',l_2,l_2') + \Sigma_{j_1j'j_2j'}^{(S',S)}(l_1,l_1',l_2,l_2')$$

in Eq. (35) can be expressed as

$$\Sigma_3^{(S',S)}(l_1,l_1',l_2,l_2') = \frac{1}{(N-1)(N-2)} \Sigma_1^{(S',S)}(l_1,l_1',l_2,l_2') - \frac{2}{N-2} \Sigma_2^{(S',S)}(l_1,l_1',l_2,l_2'), \tag{A5}$$

where

$$\Sigma_1^{(S',S)}(l_1,l_1',l_2,l_2') = \Sigma_{jj}^{(S',S)}(l_1,l_2) + \Sigma_{jj}^{(S',S)}(l_1',l_2) + \Sigma_{jj}^{(S',S)}(l_1,l_2') + \Sigma_{jj}^{(S',S)}(l_1',l_2') \tag{A6}$$

and $\Sigma_2^{(S',S)}(l_1,l_1',l_2,l_2')$ is defined by Eq. (33).

Finally, if $j_1 \neq j_2 \neq j_1'$ and $j_1 \neq j_2' \neq j_2$, the sum is expressed using the following identity:

$$\begin{aligned}\sum_{\mathcal{P}} \delta_{l_1,\mathcal{P}j_1} \delta_{l_1',\mathcal{P}j_1'} \delta_{l_2,\mathcal{R}\mathcal{P}j_2} \delta_{l_2',\mathcal{R}\mathcal{P}j_2'} &= \sum_{l_1 \neq l \neq l_1'} \delta_{l_2,\mathcal{R}l} \sum_{l_1 \neq l' \neq l_1'} \delta_{l_2',\mathcal{R}l'} \sum_{\mathcal{P}} \delta_{l_1,\mathcal{P}j_1} \delta_{l_1',\mathcal{P}j_1'} \delta_{l,\mathcal{P}j_2} \delta_{l',\mathcal{P}j_2'} \\ &= (N-4)! \sum_{l,l'} \delta_{l_2,\mathcal{R}l} \delta_{l_2',\mathcal{R}l'} \left(1 - \delta_{ll_1}\right)\left(1 - \delta_{ll_1'}\right)\left(1 - \delta_{l'l_1}\right)\left(1 - \delta_{l'l_1'}\right).\end{aligned}$$

Then $\Sigma_{j_1 j_1' j_2 j_2'}^{(S',S)}(l_1,l_1',l_2,l_2') \equiv \Sigma_4^{(S',S)}(l_1,l_1',l_2,l_2')$ [see Eq. (35)] is independent of j_1, j_2, j_1', and j_2' and

$$\begin{aligned}\Sigma_4^{(S',S)}(l_1,l_1',l_2,l_2') &= \sum_{\mathcal{R}} D_{[0][0]}^{[\lambda']}(\mathcal{R}) D_{[0][0]}^{[\lambda]}(\mathcal{R})(N-4)!(1 - \delta_{l_2,\mathcal{R}l_1} - \delta_{l_2,\mathcal{R}l_1'} - \delta_{l_2',\mathcal{R}l_1} - \delta_{l_2',\mathcal{R}l_1'} + \delta_{l_2,\mathcal{R}l_1} \delta_{l_2',\mathcal{R}l_1'} + \delta_{l_2,\mathcal{R}l_1'} \delta_{l_2',\mathcal{R}l_1}) \\ &= \frac{N!(N-4)!}{f_S} \delta_{\lambda\lambda'} - \frac{1}{(N-1)(N-2)(N-3)} \Sigma_1^{(S',S)}(l_1,l_1',l_2,l_2') + \frac{1}{(N-2)(N-3)} \Sigma_2^{(S',S)}(l_1,l_1',l_2,l_2')\end{aligned} \tag{A7}$$

[see Eqs. (I.5), (33) and (A6)]. Therefore, each sum (30) is expressed in terms of (A3) and (A4).

Let us at first calculate the sums (A3) for $S = S'$. If $l_1 = l_2 = \lambda_1 - 1$, $l'_1 = l'_2 = \lambda_1$, the Kronecker symbols in Eq. (A3) select the permutations of the form (A1) with $\mathcal{P}'$ which do not affect l_1 and l'_1 and $l_1 \neq i'_k \neq l'_1$. Therefore there are $(\lambda_1 - 2)!$ permutations $\mathcal{P}'$, $\lambda_2!$ permutations $\mathcal{P}''$, and number of distinct choices of the sets of i'_k and i''_k are given by the binomial coefficients $\binom{\lambda_1-2}{n_{ex}}$ and $\binom{\lambda_2}{n_{ex}}$, respectively. Then Eq. (A3) can be transformed as follows:

$$\Sigma^{(S,S)}_{jj'jj'}(\lambda_1-1,\lambda_1,\lambda_1-1,\lambda_1) =(N-2)! \sum_{n_{ex}=0}^{\lambda_2} (\lambda_1-2)!\lambda_2! \binom{\lambda_1-2}{n_{ex}}\binom{\lambda_2}{n_{ex}}\binom{\lambda_1}{n_{ex}}^{-2}$$

$$=\frac{N!(N-2)!}{f_S\lambda_1(\lambda_1-1)}\left[1-\frac{2\lambda_2}{(\lambda_1-1)(\lambda_1-\lambda_2+3)}+\frac{4\lambda_2}{\lambda_1(\lambda_1-1)(\lambda_1-\lambda_2+2)(\lambda_1-\lambda_2+3)}\right].$$

If $l_1 = l'_2 = \lambda_1 - 1$, $l'_1 = l_2 = \lambda_1$, the permutations

$$\mathcal{R} = \mathcal{P}_{l_1 l_2} \prod_{k=1}^{k_m} \mathcal{P}_{i'_k i''_k} \mathcal{P}'\mathcal{P}'' \tag{A8}$$

satisfy the Kronecker symbols if $\mathcal{P}'$ do not affect l_1 and l'_1 and $l_1 \neq i'_k \neq l'_1$. Since $\mathcal{P}_{l_1 l_2}$ is a transposition of symbols in the first row of the Young tableau [0], $n_{ex} = k_m$ and

$$\Sigma^{(S,S)}_{jj'jj'}(\lambda_1-1,\lambda_1,\lambda_1,\lambda_1-1) = \Sigma^{(S,S)}_{jj'jj'}(\lambda_1-1,\lambda_1,\lambda_1-1,\lambda_1)$$

If $l_1 = l_2 = \lambda_1 + 1$, $l'_1 = l'_2 = \lambda_1 + 2$, the proper permutations are given by (A1) with $\mathcal{P}''$ which do not affect l_1 and l'_1 and $l_1 \neq i''_k \neq l'_1$, and with no additional restrictions to $\mathcal{P}'$ and i'_k. There are $\lambda_1!$ permutations $\mathcal{P}'$, $(\lambda_2 - 2)!$ permutations $\mathcal{P}''$, and number of distinct choices of the sets of i'_k and i''_k are given by the binomial coefficients $\binom{\lambda_1}{n_{ex}}$ and $\binom{\lambda_2-2}{n_{ex}}$, respectively. Then

$$\Sigma^{(S,S)}_{jj'jj'}(\lambda_1+1,\lambda_1+2,\lambda_1+1,\lambda_1+2) =(N-2)! \sum_{n_{ex}=0}^{\lambda_2} \lambda_1!(\lambda_2-2)! \binom{\lambda_1}{n_{ex}}\binom{\lambda_2-2}{n_{ex}}\binom{\lambda_1}{n_{ex}}^{-2}$$

$$=\frac{N!(N-2)!}{f_S\lambda_2(\lambda_2-1)}\left[1-\frac{2}{\lambda_1-\lambda_2+3}\right].$$

If $l_1 = l'_2 = \lambda_1 + 1$, $l'_1 = l_2 = \lambda_1 + 2$, the Kronecker symbols are satisfied by the permutations (A8) with the same restrictions to $\mathcal{P}''$ and i''_k as in the previous case. Since $\mathcal{P}_{l_1 l_2}$ is a transposition of symbols in the second row of the Young tableau [0], $n_{ex} = k_m$ and

$$\Sigma^{(S,S)}_{jj'jj'}(\lambda_1+1,\lambda_1+2,\lambda_1+2,\lambda_1+1) = \Sigma^{(S,S)}_{jj'jj'}(\lambda_1+1,\lambda_1+2,\lambda_1+1,\lambda_1+2).$$

If $l_1 = \lambda_1 - 1$, $l'_1 = \lambda_1$, $l_2 = \lambda_1 + 1$, and $l'_2 = \lambda_1 + 2$, the permutations

$$\mathcal{R} = \mathcal{P}_{l_1 l_2}\mathcal{P}_{l'_1 l'_2} \prod_{k=1}^{k_m} \mathcal{P}_{i'_k i''_k} \mathcal{P}'\mathcal{P}'' \tag{A9}$$

satisfy the Kronecker symbol if $\mathcal{P}'$ do not affect l_1 and l'_1 and $l_1 \neq i'_k \neq l'_1$. If $l_2 \neq i''_k \neq l'_2$ for any k, $\mathcal{P}_{l_1 l_2}$and $\mathcal{P}_{l'_1 l'_2}$are additional transpositions between the rows of the Young tableau [0], and $n_{ex} = k_m + 2$. Otherwise, if one of i''_k is equal to l_2, $\mathcal{P}_{l_1 l_2}\mathcal{P}_{i'_k l_2} = \mathcal{P}_{i'_k l_2}\mathcal{P}_{i'_k l_1}$, $n_{ex} = k_m + 1$. By the same reason $n_{ex} = k_m + 1$ if one of i''_k is equal to l'_2. If two of i''_k are equal to l_2 and l'_2, $n_{ex} = k_m$. Then

$$\Sigma^{(S,S)}_{jj'jj'}(\lambda_1-1,\lambda_1,\lambda_1+1,\lambda_1+2) =(N-2)! \sum_{k_m=0}^{\lambda_2} (\lambda_1-2)!\lambda_2! \binom{\lambda_1-2}{k_m}\left[\binom{\lambda_2-2}{k_m}\binom{\lambda_1}{k_m+2}^{-2} + 2\binom{\lambda_2-2}{k_m-1}\binom{\lambda_1}{k_m+1}^{-2}\right.$$

$$\left.+\binom{\lambda_2-2}{k_m-2}\binom{\lambda_1}{k_m}^{-2}\right] = \frac{2N!(N-2)!}{f_S\lambda_1(\lambda_1-1)(\lambda_1-\lambda_2+2)(\lambda_1-\lambda_2+3)}.$$

This derivation is valid for the case of $l_1 = \lambda_1 - 1$, $l'_1 = \lambda_1$, $l_2 = \lambda_1 + 2$, and $l'_2 = \lambda_1 + 1$ as well, giving

$$\Sigma^{(S,S)}_{jj'jj'}(\lambda_1-1,\lambda_1,\lambda_1+2,\lambda_1+1) = \Sigma^{(S,S)}_{jj'jj'}(\lambda_1-1,\lambda_1,\lambda_1+1,\lambda_1+2).$$

Consider now the case of $S' = S - 1$. If $l_1 = l_2 = \lambda_1 - 1$, $l'_1 = l'_2 = \lambda_1$, the Kronecker symbols in Eq. (A3) select the permutations of the form (A1) with $\mathcal{P}'$ which do not affect l_1 and l'_1 and $l_1 \neq i'_k \neq l'_1$. Then

$$\Sigma^{(S-1,S)}_{jj'jj'}(\lambda_1-1,\lambda_1,\lambda_1-1,\lambda_1) = (N-2)! \sum_{n_{ex}=0}^{\lambda_2} (\lambda_1-2)!\lambda_2! \binom{\lambda_1-2}{n_{ex}}\binom{\lambda_2}{n_{ex}}\binom{\lambda_1}{n_{ex}}^{-1}\binom{\lambda_1-1}{n_{ex}}^{-1} = \frac{N!(N-2)!\left(\lambda_1^2-\lambda_1\lambda_2+\lambda_1-2\right)}{f_S\lambda_1(\lambda_1-1)^2(\lambda_1-\lambda_2+2)}.$$

If $l_1 = l_2' = \lambda_1 - 1$, $l_1' = l_2 = \lambda_1$, the permutations (A8) satisfy the Kronecker symbols if $\mathcal{P}'$ do not affect l_1 and l_1' and $l_1 \neq i_k' \neq l_1'$. Since $\mathcal{P}_{l_1 l_2}$ is an additional transposition between the rows of the Young tableau [0] of the shape $\lambda' = [\lambda_1 - 1, \lambda_2 + 1]$, $n_{\text{ex}} = k_m$ and $n_{\text{ex}}' = k_m + 1$. As a result,

$$\Sigma_{jj'jj'}^{(S-1,S)}(\lambda_1 - 1,\lambda_1,\lambda_1,\lambda_1 - 1) = -(N-2)! \sum_{k_m=0}^{\lambda_2} (\lambda_1 - 2)!\lambda_2! \binom{\lambda_1 - 2}{k_m}\binom{\lambda_2}{k_m}\binom{\lambda_1}{k_m}^{-1}\binom{\lambda_1 - 1}{k_m + 1}^{-1}$$
$$= -\frac{N!(N-2)!(\lambda_1 + 2)}{f_S \lambda_1(\lambda_1 - 1)^2(\lambda_1 - \lambda_2 + 2)}.$$

If $l_1 = l_2 = \lambda_1$, $l_1' = l_2' = \lambda_1 + 1$, the Kronecker symbols in Eq. (A3) are satisfied by the permutations of the form (A1) with $\mathcal{P}'$ which do not affect l_1, $\mathcal{P}''$ which do not affect l_1', $i_k' \neq l_1$, and $i_k'' \neq l_1'$. Then

$$\Sigma_{jj'jj'}^{(S-1,S)}(\lambda_1,\lambda_1 + 1,\lambda_1,\lambda_1 + 1) = (N-2)! \sum_{n_{\text{ex}}=0}^{\lambda_2} (\lambda_1 - 1)!(\lambda_2 - 1)! \binom{\lambda_1 - 1}{n_{\text{ex}}}\binom{\lambda_2 - 1}{n_{\text{ex}}}\binom{\lambda_1}{n_{\text{ex}}}^{-1}\binom{\lambda_1 - 1}{n_{\text{ex}}}^{-1}$$
$$= \frac{N!(N-2)!(\lambda_1 - \lambda_2 + 1)}{f_S \lambda_1 \lambda_2(\lambda_1 - \lambda_2 + 2)}.$$

If $l_1 = l_2' = \lambda_1$, $l_1' = l_2 = \lambda_1 + 1$, the permutations (A8) satisfy the Kronecker symbols if $\mathcal{P}'$ do not affect l_1, $\mathcal{P}''$ do not affect l_1', $i_k' \neq l_1$, and $i_k'' \neq l_1'$. Since $\mathcal{P}_{l_1 l_2}$ is an additional transposition between the rows of the Young tableau [0] of the shape λ, $n_{\text{ex}} = k_m + 1$ and $n_{\text{ex}}' = k_m$. As a result,

$$\Sigma_{jj'jj'}^{(S-1,S)}(\lambda_1,\lambda_1 + 1,\lambda_1 + 1,\lambda_1) = -(N-2)! \sum_{k_m=0}^{\lambda_2} (\lambda_1 - 1)!(\lambda_2 - 1)! \binom{\lambda_1 - 1}{k_m}\binom{\lambda_2 - 1}{k_m}\binom{\lambda_1}{k_m + 1}^{-1}\binom{\lambda_1 - 1}{k_m}^{-1}$$
$$= -\frac{N!(N-2)!}{f_S \lambda_1 \lambda_2(\lambda_1 - \lambda_2 + 2)}.$$

If $l_1 = \lambda_1 - 1$, $l_1' = l_2' = \lambda_1$, $l_2 = \lambda_1 + 1$, the proper permutations are given by (A8) with $\mathcal{P}'$ which do not affect l_1 and l_1' and $l_1 \neq i_k' \neq l_1'$. $\mathcal{P}_{l_1 l_2}$ is an additional transposition between the rows of the Young tableau [0] of the shapes λ and λ' and $n_{\text{ex}} = n_{\text{ex}}' = k_m + 1$, unless $i_k'' = \lambda_1 + 1$, when $n_{\text{ex}} = n_{\text{ex}}' = k_m$. Then

$$\Sigma_{jj'jj'}^{(S-1,S)}(\lambda_1 - 1,\lambda_1,\lambda_1 + 1,\lambda_1) = (N-2)! \sum_{k_m=0}^{\lambda_2} (\lambda_1 - 2)!\lambda_2! \binom{\lambda_1 - 2}{k_m}\left[\binom{\lambda_2 - 1}{k_m}\binom{\lambda_1}{k_m + 1}^{-1}\binom{\lambda_1 - 1}{k_m + 1}^{-1}\right.$$
$$\left. + \binom{\lambda_2 - 1}{k_m - 1}\binom{\lambda_1}{k_m}^{-1}\binom{\lambda_1 - 1}{k_m}^{-1}\right] = \frac{N!(N-2)!}{f_S \lambda_1(\lambda_1 - 1)(\lambda_1 - \lambda_2 + 2)}.$$

If $l_1 = \lambda_1 - 1$, $l_1' = l_2 = \lambda_1$, $l_2' = \lambda_1 + 1$, the Kronecker symbols are satisfied by the permutations (A9) with the same restrictions to $\mathcal{P}'$ and i_k' as in the previous case. Since $\mathcal{P}_{\lambda_1 \lambda_1 - 1}\mathcal{P}_{\lambda_1 \lambda_1 + 1} = \mathcal{P}_{\lambda_1 \lambda_1 + 1}\mathcal{P}_{\lambda_1 - 1 \lambda_1 + 1} n_{\text{ex}} = n_{\text{ex}}' = k_m + 1$, unless $i_k'' = \lambda_1 + 1$, when $n_{\text{ex}} = n_{\text{ex}}' = k_m$, as in the previous case, and

$$\Sigma_{jj'jj'}^{(S-1,S)}(\lambda_1 - 1,\lambda_1,\lambda_1,\lambda_1 + 1) = \Sigma_{jj'jj'}^{(S-1,S)}(\lambda_1,\lambda_1 - 1,\lambda_1,\lambda_1 + 1).$$

The last relevant case is $S' = S - 2$. If $l_1 = l_2 = \lambda_1 - 1$, $l_1' = l_2' = \lambda_1$, the Kronecker symbols in Eq. (A3) select the permutations of the form (A1) with $\mathcal{P}'$ which do not affect l_1 and l_1' and $l_1 \neq i_k' \neq l_1'$. Then

$$\Sigma_{jj'jj'}^{(S-2,S)}(\lambda_1 - 1,\lambda_1,\lambda_1 - 1,\lambda_1) = (N-2)! \sum_{n_{\text{ex}}=0}^{\lambda_2} (\lambda_1 - 2)!\lambda_2! \binom{\lambda_1 - 2}{n_{\text{ex}}}\binom{\lambda_2}{n_{\text{ex}}}\binom{\lambda_1}{n_{\text{ex}}}^{-1}\binom{\lambda_1 - 2}{n_{\text{ex}}}^{-1} = \frac{N!(N-2)!}{f_S \lambda_1(\lambda_1 - 1)}.$$

If $l_1 = l_2' = \lambda_1 - 1$, $l_1' = l_2 = \lambda_1$,the Kronecker symbols are satisfied by the permutations (A8) with the same restrictions to $\mathcal{P}'$ and i_k' as in the previous case. Now $\mathcal{P}_{l_1 l_2}$ is a transposition within the same row of the Young tableau [0] of the shapes λ or $\lambda' = [\lambda_1 - 2, \lambda_2 + 2]$. Therefore

$$\Sigma_{jj'jj'}^{(S-2,S)}(\lambda_1 - 1,\lambda_1,\lambda_1,\lambda_1 - 1) = \Sigma_{jj'jj'}^{(S-2,S)}(\lambda_1,\lambda_1 - 1,\lambda_1,\lambda_1 - 1).$$

APPENDIX B: CALCULATION OF THE SUMS (32)

The sum (32) is expressed using the relations (23) and (18) as

$$\Sigma_{j_1 j_1' j_2 j_2'}^{(S)}(l,l') = \sum_{\mathcal{P}} D_{[0][0]}^{[\lambda]}(\mathcal{P}\mathcal{P}_{j_2 j_2'}\mathcal{P}^{-1})\delta_{l,\mathcal{P}j_1}\delta_{l',\mathcal{P}j_1'}$$

Only the sums with $j_1 \neq j_1'$ and $j_2 \neq j_2'$ are used here. This implies $l \neq l'$.

If $j_1 = j_2$ and $j'_1 = j'_2$, or $j_1 = j'_2$ and $j_1 = j'_2$, there are $(N-2)!$ permutations $\mathcal{P}$ which satisfy the Kronecker symbols, and the identity (24) leads to

$$\Sigma^{(S)}_{jj'jj'}(l,l') = \Sigma^{(S)}_{jj'j'j}(l,l') = (N-2)!D^{[\lambda]}_{[0][0]}(\mathcal{P}_{ll'}).$$

Therefore

$$\Sigma^{(S)}_{jj'jj'}(\lambda_1-1,\lambda_1) = \Sigma^{(S)}_{jj'jj'}(\lambda_1+1,\lambda_1+2) = (N-2)!,$$

since l and l' are in the same row of the Young tableau [0] of the shape λ [see Eq. (I.8)]. Then

$$\Sigma^{(S)}_2(\lambda_1-1,\lambda_1) = \Sigma^{(S)}_2(\lambda_1+1,\lambda_1+2) = 2(N-2)! \tag{B1}$$

in Eq. (35).

If $j_1 = j_2$, but $j_1 \neq j'_2 \neq j'_1$,

$$\Sigma^{(S)}_{jj'_1jj'_2}(l,l') = \sum_{l\neq l''\neq l'} D^{[\lambda]}_{[0][0]}(\mathcal{P}_{ll''}) \sum_{\mathcal{P}} \delta_{l,\mathcal{P}j}\delta_{l',\mathcal{P}j'_1}\delta_{l'',\mathcal{P}j'_2} = (N-3)! \sum_{l\neq l''\neq l'} D^{[\lambda]}_{[0][0]}(\mathcal{P}_{ll''}).$$

Similarly,

$$\Sigma^{(S)}_{jj'_1j_2j}(l,l') = \Sigma^{(S)}_{j_1jj_2j}(l,l') = \Sigma^{(S)}_{j_1jjj'_2}(l,l') = \Sigma^{(S)}_{jj'_1jj'_2}(l,l').$$

If $l = \lambda_1 - 1, l' = \lambda_1$, for $l'' \leqslant \lambda_1 - 2$, l and l'' are in the same row of the Young tableau [0] of the shape λ, and $D^{[\lambda]}_{[0][0]}(\mathcal{P}_{ll''}) = 1$. For $l'' > \lambda_1$, l and l'' are in different rows of this Young tableau, and $D^{[\lambda]}_{[0][0]}(\mathcal{P}_{ll''}) = -1/\lambda_1$ [see Eq. (A2)]. Then

$$\Sigma^{(S)}_{jj'_1jj'_2}(\lambda_1-1,\lambda_1) = (N-3)!\left(\lambda_1 - 2 - \frac{\lambda_2}{\lambda_1}\right).$$

Similarly,

$$\Sigma^{(S)}_{jj'_1jj'_2}(\lambda_1+1,\lambda_1+2) = (N-3)!(\lambda_2-3).$$

Then

$$\begin{aligned}\Sigma^{(S)}_3(\lambda_1-1,\lambda_1) &= 4(N-3)!(\lambda_1-2-\lambda_2/\lambda_1),\\ \Sigma^{(S)}_3(\lambda_1+1,\lambda_1+2) &= 4(N-3)!(\lambda_2-3)\end{aligned} \tag{B2}$$

in Eq. (35).

If $j_1 \neq j_2 \neq j'_1$ and $j_1 \neq j'_2 \neq j'_1$, we have

$$\Sigma^{(S)}_{j_1j'_1j_2j'_2}(l,l') = \sum_{l\neq l''\neq l'} \sum_{l\neq l'''\neq l',l'''\neq l''} D^{[\lambda]}_{[0][0]}(\mathcal{P}_{l''l'''}) \sum_{\mathcal{P}} \delta_{l,\mathcal{P}j_1}\delta_{l',\mathcal{P}j'_1}\delta_{l'',\mathcal{P}j_2}\delta_{l''',\mathcal{P}j'_2} = (N-4)! \sum_{l\neq l''\neq l'} \sum_{l\neq l'''\neq l',l'''\neq l''} D^{[\lambda]}_{[0][0]}(\mathcal{P}_{l''l'''}).$$

Using the same values of the Young matrix elements as in the previous case, one gets

$$\begin{aligned}\Sigma^{(S)}_4(\lambda_1-1,\lambda_1) &= \Sigma^{(S)}_{j_1j'_1j_2j'_2}(\lambda_1-1,\lambda_1) = (N-4)!\left[(\lambda_1-2)(\lambda_1-3) + \lambda_2(\lambda_2-1) - 2(\lambda_1-2)\frac{\lambda_2}{\lambda_1}\right],\\ \Sigma^{(S)}_4(\lambda_1+1,\lambda_1+2) &= \Sigma^{(S)}_{j_1j'_1j_2j'_2}(\lambda_1+1,\lambda_1+2) = (N-4)![(\lambda_2-2)(\lambda_2-5) + \lambda_1(\lambda_1-1)].\end{aligned} \tag{B3}$$

APPENDIX C: CALCULATION OF THE SUMS (A4)

The sum (A4), expressed as

$$\Sigma^{(S',S)}_{jj}(l,l') = (N-1)! \sum_{\mathcal{R}} D^{[\lambda']}_{[0][0]}(\mathcal{R}) D^{[\lambda]}_{[0][0]}(\mathcal{R}) \delta_{l',\mathcal{R}l}, \tag{C1}$$

is denoted for consistency with the sum $\Sigma^{(S',S)}_{jj}$ [see Eq. (I.A1)], which is its special case for $l = l' = \lambda_1$. Since $D^{[\lambda]}_{[0][0]}(\mathcal{R}^{-1}) = D^{[\lambda]}_{[0][0]}(\mathcal{R})$ and $\delta_{l',\mathcal{R}l} = \delta_{l,\mathcal{R}^{-1}l'}$, the substitution $\mathcal{R} = \mathcal{R}^{-1}$ transposes arguments l and l'. Therefore

$$\Sigma^{(S',S)}_{jj}(l,l') = \Sigma^{(S',S)}_{jj}(l',l). \tag{C2}$$

Consider at first the case $S = S'$. If $l = l' \leqslant \lambda_1$, the Kronecker symbol in Eq. (C1) selects the permutations of the form (A1) with $\mathcal{P}'$ which do not affect l and $i'_k \neq l$. Therefore there are $(\lambda_1 - 1)!$ permutations $\mathcal{P}'$, $\lambda_2!$ permutations $\mathcal{P}''$, and number of distinct choices of the sets of i'_k and i''_k are given by the binomial coefficients $\binom{\lambda_1-1}{n_{\mathrm{ex}}}$ and $\binom{\lambda_2}{n_{\mathrm{ex}}}$, respectively. Then this sum, being independent of the particular values of l, is equal to $\Sigma_{jj}^{(S,S)}(\lambda_1,\lambda_1) \equiv \Sigma_{jj}^{(S,S)}$, calculated in the Appendix in Ref. [1],

$$\Sigma_{jj}^{(S,S)}(l,l) = \frac{N!(N-1)!}{f_S\lambda_1^2}\left[\lambda_1 - \frac{\lambda_2}{\lambda_1-\lambda_2+2}\right].$$

If $l \neq l'$, but $l \leqslant \lambda_1$ and $l' \leqslant \lambda_1$, the Kronecker symbol in Eq. (C1) selects permutations

$$\mathcal{R} = \mathcal{P}_{ll'}\prod_{k=1}^{k_m}\mathcal{P}_{i'_k i''_k}\mathcal{P}'\mathcal{P}'', \tag{C3}$$

with the same restrictions to $\mathcal{P}'$ and i'_k. Since both l and l' are in the first row of the Young tableau [0], $\Sigma_{jj}^{(S,S)}(l,l') = \Sigma_{jj}^{(S,S)}(l,l)$ in this case.

If $l = l' > \lambda_1$, the Kronecker symbol in Eq. (C1) selects the permutations (A1) with $\mathcal{P}''$ which do not affect l' and $i''_k \neq l'$. There are $\lambda_1!$ permutations $\mathcal{P}'$, $(\lambda_2-1)!$ permutations $\mathcal{P}''$, and number of distinct choices of the sets of i'_k and i''_k are given by the binomial coefficients $\binom{\lambda_1}{n_{\mathrm{ex}}}$ and $\binom{\lambda_2-1}{n_{\mathrm{ex}}}$, respectively. Then Eq. (A4) can be represented as

$$\begin{aligned}\Sigma_{jj}^{(S,S)}(l,l) &= (N-1)!\sum_{n_{\mathrm{ex}}=0}^{\lambda_2}\lambda_1!(\lambda_2-1)!\binom{\lambda_1}{n_{\mathrm{ex}}}\binom{\lambda_2-1}{n_{\mathrm{ex}}}\binom{\lambda_1}{n_{\mathrm{ex}}}^{-2} = (N-1)!((\lambda_2-1)!)^2\sum_{n_{\mathrm{ex}}=0}^{\lambda_2-1}\frac{(\lambda_1-n_{\mathrm{ex}})!}{(\lambda_2-n_{\mathrm{ex}}-1)!}\\ &= \frac{N!(N-1)!}{f_S\lambda_2}\left[1-\frac{1}{\lambda_1-\lambda_2+2}\right].\end{aligned} \tag{C4}$$

If $l \neq l'$, but $l > \lambda_1$ and $l' > \lambda_1$, the Kronecker symbol in Eq. (C1) selects permutations (C3) with the same restrictions to $\mathcal{P}''$ and i''_k as in the case of $l = l' > \lambda_1$. Since both l and l' are in the second row of the Young tableau [0], $\Sigma_{jj}^{(S,S)}(l,l') = \Sigma_{jj}^{(S,S)}(l,l)$ in this case.

If $l \leqslant \lambda_1 < l'$, the permutations (C3) satisfy the Kronecker symbol in Eq. (C1) if $\mathcal{P}'$ do not affect l and $i'_k \neq l$. If $i''_k \neq l'$ for any k, $\mathcal{P}_{ll'}$ is an additional transposition between the rows of the Young tableau [0], and $n_{\mathrm{ex}} = k_m + 1$. Otherwise, if $i''_k = l'$, since $\mathcal{P}_{ll'}\mathcal{P}_{l'i'_k} = \mathcal{P}_{li'_k}\mathcal{P}_{ll'}$, $n_{\mathrm{ex}} = k_m$. Then

$$\Sigma_{jj}^{(S,S)}(l,l') = (N-1)!\sum_{k_m=0}^{\lambda_2}(\lambda_1-1)!\lambda_2!\binom{\lambda_1-1}{k_m}\left[\binom{\lambda_2-1}{k_m}\binom{\lambda_1}{k_m+1}^{-2} + \binom{\lambda_2-1}{k_m-1}\binom{\lambda_1}{k_m}^{-2}\right] = \frac{N!(N-1)!}{f_S\lambda_1(\lambda_1-\lambda_2+2)}.$$

The next case is $S' = S-1$. If $l = l' = \lambda_1$, the sum was calculated in Appendix in Ref. [1],

$$\Sigma_{jj}^{(S-1,S)}(\lambda_1,\lambda_1) \equiv \Sigma_{jj}^{(S-1,S)} = \frac{N!(N-1)!}{f_S\lambda_1}.$$

If $l = l' = \lambda_1 - 1$, the Kronecker symbol in Eq. (C1) selects permutations

$$\mathcal{R} = \prod_{k=1}^{k_m}\mathcal{P}_{i'_k i''_k}\mathcal{P}_{\lambda_1 i_0}\mathcal{P}'\mathcal{P}'', \tag{C5}$$

if $\mathcal{P}'$ are permutations of the $\lambda_1 - 2$ first symbols, $\mathcal{P}''$ are permutations of the λ_2 last symbols, $i_0 \neq \lambda_1 - 1$, $i'_k \leqslant \lambda_1 - 2$, and $i''_k > \lambda_1$. The numbers of transpositions n_{ex} and n'_{ex} between rows of the Young tableau [0] of the shapes λ and λ', respectively, depend on i_0. If $i_0 = \lambda_1$, $n_{\mathrm{ex}}(i_0) = n'_{\mathrm{ex}}(i_0) = k_m$. If $i_0 \leqslant \lambda_1 - 2$, $n_{\mathrm{ex}}(i_0) = k_m$, $n'_{\mathrm{ex}}(i_0) = k_m + 1$, unless $i_0 = i'_k$ for any k. In the last case, $n_{\mathrm{ex}}(i_0) = k_m$ and, since $\mathcal{P}_{i'_k i''_k}\mathcal{P}_{\lambda_1 i'_k} = \mathcal{P}_{\lambda_1 i'_k}\mathcal{P}_{\lambda_1 i''_k}$, $n'_{\mathrm{ex}}(i_0) = k_m$. Similarly, if $i_0 > \lambda_1$, $n'_{\mathrm{ex}}(i_0) = k_m$, $n_{\mathrm{ex}}(i_0) = k_m + 1$, unless $i_0 = i''_k$, when $n_{\mathrm{ex}}(i_0) = k_m$. Thus for $2k_m + 1$ values of i_0 we have $n_{\mathrm{ex}}(i_0) = n'_{\mathrm{ex}}(i_0) = k_m$, for $\lambda_1 - 2 - k_m$ values $n_{\mathrm{ex}}(i_0) = k_m$, $n'_{\mathrm{ex}}(i_0) = k_m + 1$, and for $\lambda_2 - k_m$ values $n_{\mathrm{ex}}(i_0) = k_m + 1$, $n'_{\mathrm{ex}}(i_0) = k_m$. Then the sum (A4) is expressed as

$$\begin{aligned}\Sigma_{jj}^{(S-1,S)}(\lambda_1-1,\lambda_1-1) &= (N-1)!\sum_{k_m=0}^{\lambda_2}(\lambda_1-2)!\lambda_2!\binom{\lambda_1-2}{k_m}\binom{\lambda_2}{k_m}\left[(2k_m+1)\binom{\lambda_1}{k_m}^{-1}\binom{\lambda_1-1}{k_m}^{-1}\right.\\ &\left.\quad-(\lambda_1-2-k_m)\binom{\lambda_1}{k_m}^{-1}\binom{\lambda_1-1}{k_m+1}^{-1} - (\lambda_2-k_m)\binom{\lambda_1}{k_m+1}^{-1}\binom{\lambda_1-1}{k_m}^{-1}\right] = \frac{N!(N-1)!}{f_S\lambda_1(\lambda_1-1)^2}.\end{aligned}$$

If $l = \lambda_1$, $l' = \lambda_1 - 1$, the Kronecker symbol in Eq. (C1) selects permutations (C3) if $\mathcal{P}'$ are permutations of the $\lambda_1 - 1$ first symbols, $\mathcal{P}''$ are permutations of the λ_2 last symbols, $i'_k \leqslant \lambda_1 - 1$, and $i''_k > \lambda_1$. Now $n_{\mathrm{ex}} = k_m$, $n'_{\mathrm{ex}} = k_m + 1$ unless $i'_k = \lambda_1 - 1$

for any k, when $n_{\rm ex} = n'_{\rm ex} = k_m$. Then

$$\Sigma_{jj}^{(S-1,S)}(\lambda_1,\lambda_1-1) = (N-1)!\sum_{k_m=0}^{\lambda_2}(\lambda_1-1)!\lambda_2!\binom{\lambda_2}{k_m}\binom{\lambda_1}{k_m}^{-1}\left[\binom{\lambda_1-2}{k_m-1}\binom{\lambda_1-1}{k_m}^{-1} - \binom{\lambda_1-2}{k_m}\binom{\lambda_1-1}{k_m+1}^{-1}\right]$$
$$= -\frac{N!(N-1)!}{f_S\lambda_1(\lambda_1-1)}.$$

A general relation can be derived for $l \geqslant \lambda_1+1$ and arbitrary l', when the Kronecker symbol in Eq. (C1) is satisfied by

$$\mathcal{R} = \mathcal{P}_{l'N}\mathcal{P}\mathcal{P}_{lN} \tag{C6}$$

with arbitrary $\mathcal{P} \in \mathcal{S}_{N-1}$, such that $\mathcal{P}N = N$. Then $D^{[\lambda]}_{[0][0]}(\mathcal{R}) = D^{[\lambda]}_{[0][0]}(\mathcal{P}_{l'N}\mathcal{P})$, since both l and N are in the second row of the Young tableau [0] of the shape λ [see Eq. (I.8)]. If $S' < S$ and $\lambda'_1 < \lambda_1$, $D^{[\lambda']}_{[0][0]}(\mathcal{R}) = D^{[\lambda']}_{[0][0]}(\mathcal{P}_{l'N}\mathcal{P})$ by the same reason. Using Eq. (23), the sum can be expressed as

$$\Sigma_{jj}^{(S',S)}(l,l') = (N-1)!\sum_{r,r'} D^{[\lambda]}_{[0]r}(\mathcal{P}_{l'N})D^{[\lambda']}_{[0]r'}(\mathcal{P}_{l'N})\sum_{\mathcal{P}\in\mathcal{S}_{N-1}} D^{[\lambda]}_{r[0]}(\mathcal{P})D^{[\lambda']}_{r'[0]}(\mathcal{P}).$$

As $\mathcal{P}$ are elements of the subgroup $\mathcal{S}_{N-1}$ of permutations of $N-1$ first symbols, a reduction to subgroup (see [4]) can be used, $D^{[\lambda]}_{rt}(\mathcal{P}) = D^{[\bar\lambda]}_{\bar r\bar t}(\mathcal{P})$, where the Young tableaux $\bar r$ and $\bar t$, corresponding to the same Young diagram $\bar\lambda$, are obtained by the removal of the symbol N from the tableaux r and t, respectively. ($D^{[\lambda]}_{rt}(\mathcal{P}) = 0$ if $\bar r$ and $\bar t$ correspond to different Young diagrams due to different placement of the symbol N in r and t.) The summation over $\mathcal{P}$ can be then performed using the orthogonality relation (see [4,5])

$$\sum_{\mathcal{Q}\in\mathcal{S}_{N-1}} D^{[\bar\lambda']}_{\bar t'\bar r'}(\mathcal{Q})D^{[\bar\lambda]}_{\bar t\bar r}(\mathcal{Q}) = \frac{N!}{f_{\bar\lambda_1-\bar\lambda_2}(N-1)}\delta_{\bar t\bar t'}\delta_{\bar r\bar r'}\delta_{\bar\lambda\bar\lambda'}, \tag{C7}$$

where $f_S(N-1)$ is the representation dimension for $N-1$ particles. The symbol N is placed in the end of the second row in the Young tableau [0]. Therefore, $\bar\lambda = [\lambda_1,\lambda_2-1]$, $\bar\lambda' = [\lambda'_1,\lambda'_2-1]$, and $\bar\lambda = \bar\lambda'$ only if $\lambda_1 = \lambda'_1$, or $S = S'$. As a result,

$$\Sigma_{jj}^{(S',S)}(l,l') \propto \delta_{\bar\lambda\bar\lambda'} = 0$$

whenever $l \geqslant \lambda_1+1$ and $S' < S$. Due to Eq. (C2), the sum vanish whenever $l' \geqslant \lambda_1+1$ for arbitrary l too. This general relation provides the sums appearing in the present calculations

$$\Sigma_{jj}^{(S-1,S)}(\lambda_1-1,\lambda_1+1) = \Sigma_{jj}^{(S-1,S)}(\lambda_1,\lambda_1+1) = \Sigma_{jj}^{(S-1,S)}(\lambda_1+1,\lambda_1) = \Sigma_{jj}^{(S-1,S)}(\lambda_1+1,\lambda_1+1) = 0.$$

Another general relation restricts difference between S and S'. Equations (23), (C6), and the reduction to subgroup lead to $D^{[\lambda]}_{[0][0]}(\mathcal{R}) = \sum_{r,t} D^{[\lambda]}_{[0]r}(\mathcal{P}_{l'N})D^{[\bar\lambda]}_{\bar r\bar t}(\mathcal{P})D^{[\lambda]}_{t[0]}(\mathcal{P}_{lN})$ and $D^{[\lambda']}_{[0][0]}(\mathcal{R}) = \sum_{r,t} D^{[\lambda']}_{[0]r'}(\mathcal{P}_{l'N})D^{[\bar\lambda']}_{\bar r'\bar t'}(\mathcal{P})D^{[\lambda']}_{t'[0]}(\mathcal{P}_{lN})$. Then the sum (C1) contains

$$\sum_{\mathcal{P}\in\mathcal{S}_{N-1}} D^{[\bar\lambda']}_{\bar t'\bar r'}(\mathcal{P})D^{[\bar\lambda]}_{\bar t\bar r}(\mathcal{P}) \propto \delta_{\bar\lambda\bar\lambda'}$$

[see Eq. (C7)]. Now the symbol N can be placed in the end of either row of the Young tableau. Then both $\bar\lambda = [\lambda_1,\lambda_2-1]$ and $\bar\lambda = [\lambda_1-1,\lambda_2]$ are allowed, as well as two similar $\bar\lambda'$. Therefore, $|\lambda_1-\lambda'_1| \leqslant 1$, or $|S-S'| \leqslant 1$. This provides the sums appearing in the present calculations

$$\Sigma_{jj}^{(S-2,S)}(\lambda_1-1,\lambda_1-1) = \Sigma_{jj}^{(S-2,S)}(\lambda_1-1,\lambda_1) = \Sigma_{jj}^{(S-2,S)}(\lambda_1,\lambda_1-1) = \Sigma_{jj}^{(S-2,S)}(\lambda_1,\lambda_1) = 0.$$

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