Sum rules for spin-1/2 quantum gases in states with well-defined spins: Spin-independent interactions and spin-dependent external fields

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Analytical expressions are derived for sums of matrix elements and their squared moduli over 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. For spin-dependent one-body interactions with external fields and spin-independent two-body ones between the particles, the sum dependence on the many-body states is given by universal factors, which are independent of the interaction details and Hamiltonians of noninteracting particles. The sum rules are applied to perturbative analysis of energy spectra.

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I. INTRODUCTION

Calculations of quantum-mechanical system properties require matrix elements between its states. For complex systems, even a calculation of the matrix elements can constitute a complicated problem. However, in certain cases, sum rules can be derived from general principles, providing analytical expressions for sums of matrix elements or their products. The Thomas-Reiche-Kuhn and the Bethe sum rules were obtained at early years of quantum mechanics. These and similar rules (see [1]) are formulated for weighted sums of oscillator strengths, which are proportional to squared moduli of transition matrix elements, over certain sets of eigenstates. The rules were applied to radiative transitions and scattering problems. Sum rules for dynamic structure factors (see [2]) are employed to obtain information on collective behavior of many-body systems. Various sum rules are also used in nuclear and solid-state physics, as well as in quantum field theory.

The present work derives sum rules for many-body systems of indistinguishable spinor 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 particle 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.

Many-body states of spinor particles can be described in two ways (see [3]). In the first one, 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. (19) in Sec. II below]. The second approach is based on collective spin and spatial wave functions. These wave functions depend on spins or coordinates, respectively, of all particles and form representations of the symmetric group (see [4–7]). In the case of spin-$\frac{1}{2}$ particles, the representation is unambiguously related to the total many-body spin. If the total spin is less than the maximal allowed one ($N/2$ for N particles), the wave functions belong to multidimensional, non-Abelian, irreducible representations of the symmetric group (see [4–7]), beyond the conventional paradigm of symmetric-antisymmetric functions. The symmetric or antisymmetric total wave function—such functions only are allowed by the Pauli exclusion principle—is represented as a sum of products of the spin and spatial wave functions [see Eq. (2) in Sec. II below].

In the case of noninteracting particles in spin-independent potentials, all states with the given set of spatial quantum numbers are energy-degenerate and the two kinds of wave functions are applicable, related by a linear transformation. The effect of spin-independent interactions between particles was analyzed by Heitler [8] using the theory of the symmetric group irreducible representations. That work demonstrates that the average energy of states within given irreducible representation is proportional to a certain sum of the representation characters. The character dependence on the representation lifts the degeneracy of states related to different representations, and the wave functions with defined individual spin projections become inapplicable. It is a generalization of the well-known energy splitting between the singlet and triplet states in two-electron problems.

Although the derivation [8], being done in the early years of quantum mechanics, did not take into account spin degrees of freedom and supposed that total wave functions can have arbitrary permutation symmetry, the results remain valid for symmetric or antisymmetric total wave functions, composed from spin and spatial functions of arbitrary symmetry. Matrix elements of spin-independent Hamiltonians between the latter wave functions can be reduced to the matrix elements between spatial wave functions due to orthogonality of the spin wave functions (see Sec. IV). Besides justification of the Heitler results, this reduction provides the basis for spin-free quantum chemistry (see [6,7])—the method of calculations of energies and other properties of atoms and molecules.

Spinor quantum gases are intensively studied starting from the first experimental [9,10] and theoretical [11,12] works (see book [2], reviews [13,14], and references therein). The collective spin and spatial wave functions were used in the derivation of exact quantum solutions for one-dimensional homogeneous gas [15,16] and in analyses of selection rules and correlations [17]. SU(M)-symmetric gases, introduced in Refs. [18–20] and recently observed in Refs. [21,22], are described in a similar way [19], where the total wave function is composed of spin and electronic functions.

Other forms of many-body wave functions with defined total spin have been employed as well. The Lieb-Mattis theorem for ordering of energy levels in fermionic systems

has been derived in Ref. [23]. One-dimensional gas of spin-$\frac{1}{2}$ fermions in arbitrary potential has been analyzed for hard-core zero-range interactions in Ref. [24], where an exact solution was derived, and for zero-range interactions of arbitrary strength in Ref. [25], where qualitative properties of energy spectra are presented. An exact solution for one-dimensional hard-core Bose-Fermi mixture was derived in Ref. [26]. Intersystem degeneracies in spin-$\frac{1}{2}$ Fermi gases and energy spectra for certain few-body systems have been obtained in Ref. [27]. Symmetries of trapped and interacting bosons and fermions and qualitative behavior of the energy spectra at intermediate interaction strengths were analyzed in Refs. [28,29].

The sum of matrix elements of spin-independent interparticle interactions directly follows from the Heitler results [8]. The present paper provides the sums of squared moduli of these matrix elements, as well as sums of matrix elements and their squared moduli for spin-dependent external fields. Such fields can be used for transfer of population between states with different total spins, as described in [17]. Besides, spin-changing matrix elements can provide an estimate of stability of the well-defined-spin states.

Section II sets the analyzed problem and provides representations of spin, spatial, and total wave functions for separable spin and spatial degrees of freedom and for noninteracting particles. Wave functions with defined particle spin projections are discussed in this section too. Section III contains derivation of the sum rules. Matrix elements of spin-dependent external fields for different total spin projections are related using the Wigner-Eckart theorem. Then sums of these matrix elements and their squared moduli are calculated for the maximal allowed spin projections. Sum rules for spin-independent interactions between particles are provided in Sec. IV. The sum rules are applied to description of the shifts and splittings of energy levels in Sec. V. The quantitative properties of energy spectra are provided for an arbitrary number of particles in the regime of weak interactions using perturbation theory. The Appendix contains calculation of sums, used in Sec. III.

II. HAMILTONIAN AND WAVE FUNCTIONS

Consider a system of N particles with the Hamiltonian

$$\hat{H} = \hat{H}_{\rm spat} + \hat{H}_{\rm spin} \tag{1}$$

being a sum of the spin-independent $\hat{H}_{\rm spat}$ and coordinate-independent $\hat{H}_{\rm spin}$. Each of $\hat{H}_{\rm spat}$ and $\hat{H}_{\rm spin}$ is permutation-invariant.

The total wave function is expressed in the form

$$\Psi^{(S)}_{nl} = f_S^{-1/2} \sum_t \Phi^{(S)}_{tn} \Xi^{(S)}_{tl}. \tag{2}$$

Here spatial $\Phi^{(S)}_{tn}$ and spin $\Xi^{(S)}_{tl}$ functions form bases of irreducible representations of the symmetric group $\mathcal{S}_N$ of N-symbol permutations [4–7]. This means that a permutation $\mathcal{P}$ of the particles transforms each function to a linear combination of functions in the same representation,

$$\mathcal{P}\Phi^{(S)}_{tn} = {\rm sgn}(\mathcal{P}) \sum_{t'} D^{[\lambda]}_{t't}(\mathcal{P}) \Phi^{(S)}_{t'n},$$

$$\mathcal{P}\Xi^{(S)}_{tl} = \sum_{t'} D^{[\lambda]}_{t't}(\mathcal{P}) \Xi^{(S)}_{t'l}.$$

Here the factor ${\rm sgn}(\mathcal{P})$ is the permutation parity for fermions and ${\rm sgn}(\mathcal{P}) \equiv 1$ is for bosons. This factor provides the proper permutation symmetry of the total wave function

$$\mathcal{P}\Psi^{(S)}_{nl} = {\rm sgn}(\mathcal{P}) \Psi^{(S)}_{nl}. \tag{3}$$

The matrices of the Young orthogonal representation [4–7] $D^{[\lambda]}_{t't}(\mathcal{P})$ of the symmetric group $\mathcal{S}_N$ are associated with the two-row Young diagrams $\lambda = [N/2+S, N/2-S]$, which are unambiguously related to the total spin S. Different representations, associated with the same Young diagram, are labeled by multi-indices n and l for the spatial and spin functions, respectively. The representation basis functions are labeled by the standard Young tableaux t and t' of the shape λ. The dimension of the representation is equal to the number of different tableaux,

$$f_S = \frac{N!(2S+1)}{(N/2+S+1)!(N/2-S)!}. \tag{4}$$

If $S = N/2$, $f_S = 1$, $D^{[\lambda]}_{t't}(\mathcal{P}) = 1$, and the functions $\Phi^{(S)}_{tn}$ and $\Xi^{(S)}_{tl}$ remain unchanged on permutations of particles or change their sign ($\Phi^{(S)}_{tn}$ for fermions). Otherwise, the functions belong to multidimensional, non-Abelian irreducible representations of the symmetric group. For example, the states of $N = 3$ particles with $S = 1/2$ are associated with the Young diagram $[2,1]$ and there are $f_S = 2$ standard Young tableaux with the Yamanouchi symbols (see [4,5]) $(2,1,1)$ and $(1,2,1)$.

The Young orthogonal matrices obey the orthogonality relation [6,7]

$$\sum_{\mathcal{P}} D^{[\lambda']}_{t'r'}(\mathcal{P}) D^{[\lambda]}_{tr}(\mathcal{P}) = \frac{N!}{f_S} \delta_{tt'} \delta_{rr'} \delta_{\lambda\lambda'}, \tag{5}$$

the general relation for representation matrices,

$$\sum_t D^{[\lambda]}_{r't}(\mathcal{P}) D^{[\lambda]}_{tr}(\mathcal{Q}) = D^{[\lambda]}_{r'r}(\mathcal{P}\mathcal{Q}), \tag{6}$$

and the relation for orthogonal matrices,

$$D^{[\lambda]}_{tr}(\mathcal{P}^{-1}) = D^{[\lambda]}_{rt}(\mathcal{P}). \tag{7}$$

Additional relations can be obtained for elements of the first column $D^{[\lambda]}_{t[0]}(\mathcal{P})$ of the Young orthogonal matrices. Here [0] is the first Young tableau, in which the symbols are arranged by rows in the sequence of natural numbers. For example, the Young tableaux [0] have Yamanouchi symbols $(2,1,1)$, $(2,2,1,1)$, and $(2,1,1,1)$ for the Young diagrams $[2,1]$, $[2^2]$, and $[3,1]$, respectively. Each permutation involving symbols between $j_{\rm min}$ and $j_{\rm max}$ can be written as a product of elementary transpositions $\mathcal{P}_{jj+1}$ with $j_{\rm min} \leqslant j < j_{\rm max}$ (see [5–7]). According to the Young orthogonal matrix calculation rules (see [5–7]), $D^{[\lambda]}_{rt}(\mathcal{P}_{jj+1}) = \delta_{rt}$ if j and $j+1$ are in the same row of the Young tableau t. Then Eq. (6) leads to $D^{[\lambda]}_{t[0]}(\mathcal{P}) = \delta_{t[0]}$ if the permutation $\mathcal{P}$ involves the symbols in one row only and can be, therefore, written as a product of

elementary transpositions of symbols in the same row. Let $\mathcal{P}'$ and $\mathcal{P}''$ be, respectively, arbitrary permutations of the symbols in the first and in the second row of the Young tableau [0], which do not permute symbols between the rows. Then we get, using Eq. (6),

$$D^{[\lambda]}_{t[0]}(\mathcal{P}\mathcal{P}'\mathcal{P}'') = \sum_r D^{[\lambda]}_{tr}(\mathcal{P}) D^{[\lambda']}_{r[0]}(\mathcal{P}'\mathcal{P}'') = D^{[\lambda]}_{t[0]}(\mathcal{P}). \quad (8)$$

The spatial and spin wave functions form orthonormal basis sets,

$$\left\langle \Phi^{(S')}_{t'n'} \middle| \Phi^{(S)}_{tn} \right\rangle = \delta_{S'S}\delta_{t't}\delta_{n'n}, \quad (9)$$

$$\left\langle \Xi^{(S')}_{t'l'} \middle| \Xi^{(S)}_{tl} \right\rangle = \delta_{S'S}\delta_{t't}\delta_{l'l}. \quad (10)$$

The spatial functions of noninteracting particles are expressed as [6,7]

$$\tilde{\Phi}^{(S)}_{tr\{n\}} = \left(\frac{f_S}{N!}\right)^{1/2} \sum_{\mathcal{P}} \mathrm{sgn}(\mathcal{P}) D^{[\lambda]}_{tr}(\mathcal{P}) \prod_{j=1}^{N} \varphi_{n_j}(\mathbf{r}_{\mathcal{P}j}) \quad (11)$$

in terms of the spatial orbitals—the eigenfunctions $\varphi_n(\mathbf{r})$ of the one-body Hamiltonian of noninteracting particle $\hat{H}_0(j)$,

$$\hat{H}_0(j)\varphi_n(\mathbf{r}_j) = \varepsilon_n \varphi_n(\mathbf{r}_j), \quad (12)$$

where $\mathbf{r}_j$ is the D-dimensional coordinate of the jth particle (D can be either 1, 2, or 3 in real physical systems). The representation is determined by the set of the spatial quantum numbers $\{n\}$ and the Young tableau r, which can take one of f_S values. Then the multi-index n is specifically chosen as $r\{n\}$. All quantum numbers n_j in the set $\{n\}$ are supposed to be different. This situation takes place in nondegenerate gases, when probabilities of multiple occupation of spatial states are negligibly small, although the multiple occupation is not forbidden by itself. Another example is an optical lattice in the unit-filling regime [17].

The functions (11) satisfy the Schrödinger equation

$$\sum_{j=1}^{N} \hat{H}_0(j)\tilde{\Phi}^{(S)}_{tr\{n\}} = \sum_{j=1}^{N} \varepsilon_{n_j} \tilde{\Phi}^{(S)}_{tr\{n\}}.$$

Their eigenenergies are independent of r. Therefore, there are f_S degenerate states of noninteracting particles for each set $\{n\}$. The tilde denotes wave functions corresponding to the spatial Hamiltonian without interactions between particles. Then Eq. (2) gives us the total wave functions of particles with no coordinate-dependent interactions,

$$\tilde{\Psi}^{(S)}_{r\{n\}l} = f_S^{-1/2} \sum_t \tilde{\Phi}^{(S)}_{tr\{n\}} \Xi^{(S)}_{tl}. \quad (13)$$

In the absence of interactions between spins, the spin wave functions are eigenfunctions of the total spin projection operator $\hat{S}_z$ and can be expressed as

$$\Xi^{(S)}_{tS_z} = C_{SS_z} \sum_{\mathcal{P}} D^{[\lambda]}_{t[0]}(\mathcal{P}) \prod_{j=1}^{N/2+S_z} |\uparrow(\mathcal{P}j)\rangle \times \prod_{j=N/2+S_z+1}^{N} |\downarrow(\mathcal{P}j)\rangle. \quad (14)$$

Here the multi-index l is specifically chosen as the total spin projection S_z. In the case of the spin wave function, each of two spin states, $|\uparrow\rangle$ and $|\downarrow\rangle$, has to be occupied by several particles, if $N > 2$. Hence the normalization factor [30]

$$C_{SS_z} = \frac{1}{(N/2+S_z)!(N/2-S)!} \times \sqrt{\frac{(2S+1)(S+S_z)!}{(N/2+S+1)(2S)!(S-S_z)!}} \quad (15)$$

differs from the one in the spatial wave function (11). Besides, the Young tableau r can take now only the value of [0]. As a result, only one representation is associated with given total spin S and its projection S_z. The total wave function with the defined S_z is then expressed as

$$\Psi^{(S)}_{nS_z} = f_S^{-1/2} \sum_t \Phi^{(S)}_{tn} \Xi^{(S)}_{tS_z}. \quad (16)$$

In combination with the spatial wave function (11), the spin wave functions lead to the total wave functions of noninteracting particles,

$$\tilde{\Psi}^{(S)}_{r\{n\}S_z} = f_S^{-1/2} \sum_t \tilde{\Phi}^{(S)}_{tr\{n\}} \Xi^{(S)}_{tS_z} \quad (17)$$

(again, the tilde denotes that the wave functions involve spatial orbitals $\varphi_n(\mathbf{r})$ of noninteracting particles). There are f_S wave functions, labeled by the Young tableau r, having the total spin S and the set of spatial quantum numbers $\{n\}$. Then the total number of wave functions with the given total spin projection S_z will be

$$\sum_{S=S_z}^{N/2} f_S = N!/[(N/2+S_z)!(N/2-S_z)!]. \quad (18)$$

In the alternative approach, mentioned in Introduction, each particle has a given spin projection and the total many-body wave function is represented as (see [3])

$$\tilde{\Psi}_{\{n\}\{\sigma\}} = (N!)^{-1/2} \sum_{\mathcal{P}} \mathrm{sgn}(\mathcal{P}) \prod_{j=1}^{N} \varphi_{n_j}(\mathbf{r}_{\mathcal{P}j}) |\sigma_j(\mathcal{P}j)\rangle, \quad (19)$$

where the spin projection σ_j can be either $\uparrow$ or $\downarrow$ and given total spin projection S_z, the set $\{\sigma\}$ contains $N/2+S_z$ spins $\uparrow$ and $N/2-S_z$ spins $\downarrow$. For a fixed set of spatial quantum numbers $\{n\}$, the number of such states is the number of distinct choices of $N/2+S_z$ particles with spin up, and is then equal to the number (18) of the states (17). Then the sets of degenerate states $\tilde{\Psi}^{(S)}_{r\{n\}S_z}$ and $\tilde{\Psi}_{\{n\}\{\sigma\}}$ can be related by a unitary transformation. For interacting particles, the energy degeneracy of states $\tilde{\Psi}^{(S)}_{r\{n\}S_z}$ is lifted, as shown by Heitler [8] and will be discussed in Sec. V, and such transformation becomes impossible.

III. SUM RULES FOR ONE-BODY INTERACTIONS

A. Spin-projection dependence

Permutation-invariant interactions of particles with external fields can be expressed in terms of the spherical scalar

$$\hat{U} = \sum_j U(\mathbf{r}_j) \tag{20}$$

and three spherical vector components

$$\hat{U}_0 = \sum_j U(\mathbf{r}_j)\hat{s}_z(j), \quad \hat{U}_{\pm 1} = \mp\frac{1}{\sqrt{2}}\sum_j U(\mathbf{r}_j)\hat{s}_\pm(j), \tag{21}$$

(see [31]). Here

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

is the z component of the spin and

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

are the spin raising and lowering operators for the jth particle. The interaction $\hat{U}_0$ conserves the z projection of the total many-body spin, while $\hat{U}_{\pm 1}$ raises or lowers it. The interaction of the spin-up or spin-down state can be expressed in terms of $\hat{U}_0$ and the scalar $\hat{U}$,

$$\begin{aligned}\hat{U}_\uparrow &\equiv \sum_j U(\mathbf{r}_j)|\uparrow(j)\rangle\langle\uparrow(j)| = \hat{U}_0 + \frac{1}{2}\hat{U},\\ \hat{U}_\downarrow &\equiv \sum_j U(\mathbf{r}_j)|\downarrow(j)\rangle\langle\downarrow(j)| = -\hat{U}_0 + \frac{1}{2}\hat{U}.\end{aligned} \tag{22}$$

Consider matrix elements of the spherical vector and scalar interactions between eigenfunctions (16) of $\hat{S}_z$. Their dependence on S_z follows from the Wigner-Eckart theorem (see [32]). The matrix elements of the spherical scalar (20) are diagonal in spins and independent of the spin projection,

$$\left\langle \Psi^{(S')}_{n'S'_z}\middle|\hat{U}\middle|\Psi^{(S)}_{nS_z}\right\rangle = \delta_{SS'}\delta_{S_zS'_z}\left\langle \Psi^{(S)}_{n'S}\middle|\hat{U}\middle|\Psi^{(S)}_{nS}\right\rangle.$$

According to the Wigner-Eckart theorem, the matrix elements of the spherical vector components (21) can be factorized into the $3j$-Wigner symbols and the reduced matrix elements

$$\begin{aligned}&\left\langle \Psi^{(S')}_{n'S'_z}\middle|\hat{U}_k\middle|\Psi^{(S)}_{nS_z}\right\rangle\\ &\quad= (-1)^{S'-S'_z}\begin{pmatrix} S' & 1 & S\\ -S'_z & k & S_z\end{pmatrix}\langle n',S'||\hat{U}||n,S\rangle.\end{aligned}$$

Then the reduced matrix elements are expressed in terms of the matrix elements of $\hat{U}_k$ for the maximal allowed spin projection

$$\begin{aligned}&\langle n',S'||\hat{U}||n,S\rangle\\ &\quad= \begin{pmatrix} S' & 1 & S\\ -S' & S'-S & S\end{pmatrix}^{-1}\left\langle \Psi^{(S')}_{n'S'}\middle|\hat{U}_{S'-S}\middle|\Psi^{(S)}_{nS}\right\rangle,\end{aligned}$$

and the matrix elements with arbitrary spin projections can be expressed as

$$\left\langle \Psi^{(S')}_{n'S'_z}\middle|\hat{U}_k\middle|\Psi^{(S)}_{nS_z}\right\rangle = \delta_{S'_zS_z+k}X^{(S,S',1)}_{S_zk}\left\langle \Psi^{(S')}_{n'S'}\middle|\hat{U}_{S'-S}\middle|\Psi^{(S)}_{nS}\right\rangle \tag{23}$$

with the factors

$$\begin{aligned}X^{(S,S',q)}_{S_zk} &= (-1)^{S'-S_z-k}\begin{pmatrix} S & S' & q\\ S_z & -S_z-k & k\end{pmatrix}\\ &\quad\times\begin{pmatrix} S & S' & q\\ S & -S' & S'-S\end{pmatrix}^{-1}\end{aligned}$$

TABLE I. Coefficients $X^{(S,S',1)}_{S_zk}$ in Eq. (23).

k	$S-S'$	
	0	1
-1	$\frac{\sqrt{(S-S_z+1)(S+S_z)}}{\sqrt{2}S}$	$\sqrt{\frac{(S+S_z-1)(S+S_z)}{2S(2S-1)}}$
0	$\frac{S_z}{S}$	$-\sqrt{\frac{S^2-S_z^2}{S(2S-1)}}$
1	$-\frac{\sqrt{(S-S_z)(S+S_z+1)}}{\sqrt{2}S}$	$\sqrt{\frac{(S-S_z-1)(S-S_z)}{2S(2S-1)}}$

Here $S' \leqslant S$ and, according to the properties of the $3j$-Wigner symbols, the matrix elements (23) vanish if $|S-S'|>1$ (in agreement to the selection rules [17]). Values of nonvanishing coefficients, calculated with the $3j$-Wigner symbols [3,32], are presented in Table I. The Hermitian conjugate of Eq. (23), together with relations $\hat{U}_{+1} = -\hat{U}^\dagger_{-1}$ and $\hat{U}_0 = \hat{U}^\dagger_0$, gives us the matrix elements for $S' = S+1$.

Thus, each matrix element of a spin-dependent one-body interaction with an external field is related to matrix elements for the maximal allowed spin projections, which will be evaluated in the next section.

B. Matrix elements for noninteracting particles

Matrix elements of the spherical scalar (20) can be evaluated exactly for general spin wave functions. Due to the orthogonality of the spin wave functions (10), the matrix elements are diagonal in spin quantum numbers and can be reduced to the matrix elements between spatial wave functions,

$$\begin{aligned}&\left\langle \tilde{\Psi}^{(S')}_{r'\{n'\}l'}\middle|\hat{U}\middle|\tilde{\Psi}^{(S)}_{r\{n\}l}\right\rangle\\ &\quad= \delta_{SS'}\delta_{ll'}\frac{1}{f_S}\sum_t\sum_i\left\langle \tilde{\Phi}^{(S)}_{tr'\{n'\}}\middle|U(\mathbf{r}_i)\middle|\tilde{\Phi}^{(S)}_{tr\{n\}}\right\rangle.\end{aligned} \tag{24}$$

Let us calculate the spatial matrix element for the general case, $S \neq S'$, having in mind further analysis of spherical vectors. Equations (11) and (7) lead to

$$\begin{aligned}&\left\langle \tilde{\Phi}^{(S')}_{t'r'\{n'\}}\middle|U(\mathbf{r}_i)\middle|\tilde{\Phi}^{(S)}_{tr\{n\}}\right\rangle\\ &\quad= \frac{\sqrt{f_Sf_{S'}}}{N!}\sum_{\mathcal{R},\mathcal{Q}}\mathrm{sgn}(\mathcal{Q})D^{[\lambda']}_{r't'}(\mathcal{Q})\mathrm{sgn}(\mathcal{R})D^{[\lambda]}_{rt}(\mathcal{R})\\ &\qquad\times\left\langle \varphi_{n'_{\mathcal{Q}i}}\middle|U(\mathbf{r}_i)\middle|\varphi_{n_{\mathcal{R}i}}\right\rangle\prod_{i'\neq i}\delta_{n'_{\mathcal{Q}i'},n_{\mathcal{R}i'}}.\end{aligned}$$

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 one spatial quantum number remain unchanging. Supposing that the unchanged $n_{j'}$ are in the same positions in the sets $\{n\}$ and $\{n'\}$, one can see that the Kronecker symbols lead to $\mathcal{Q} = \mathcal{R}$, and, therefore,

$$\begin{aligned}&\left\langle \tilde{\Phi}^{(S')}_{t'r'\{n'\}}\middle|U(\mathbf{r}_i)\middle|\tilde{\Phi}^{(S)}_{tr\{n\}}\right\rangle\\ &\quad= \frac{\sqrt{f_Sf_{S'}}}{N!}\sum_{\mathcal{R}}D^{[\lambda']}_{r't'}(\mathcal{R})D^{[\lambda]}_{rt}(\mathcal{R})\langle n'_{\mathcal{R}i}|U|n_{\mathcal{R}i}\rangle\prod_{j'\neq\mathcal{R}i}\delta_{n'_{j'},n_{j'}},\end{aligned} \tag{25}$$

where $\langle n'|U|n\rangle = \int d^D r \varphi^*_{n'}(\mathbf{r}) U(\mathbf{r}) \varphi_n(\mathbf{r})$. Then, substituting this expression into (24), using (6), (7), and the property of representations $D^{[\lambda]}_{r'r}(\mathcal{E}) = \delta_{r'r}$, where $\mathcal{E}$ is the identity permutation, one finally gets

$$\left\langle \tilde{\Psi}^{(S')}_{r'\{n'\}l'} \middle| \hat{U} \middle| \tilde{\Psi}^{(S)}_{r\{n\}l} \right\rangle = \delta_{SS'}\delta_{ll'}\delta_{r'r} \sum_{j=1}^{N} \langle n'_j|U|n_j\rangle \prod_{j'\neq j} \delta_{n'_{j'},n_{j'}}, \tag{26}$$

It is a special case of the matrix elements obtained by Heitler [8] and Kaplan [6].

For the spherical vector interactions (21), the matrix elements cannot be represented in so simple a form. However, rather simple expressions can be derived for sums and sums of squared moduli of the matrix elements between eigenfunctions of $\hat{S}_z$. It is enough to consider matrix elements of $\hat{U}_{-1}$ and the spin-up state interaction $\hat{U}_\uparrow$ for the maximal allowed spin projection, $S'_z = S', S_z = S$, as Eq. (22) and the Wigner-Eckart theorem (23) relate to them each matrix element of each interaction. In the basis of the noninteracting particle wave functions (17), the matrix elements of $\hat{U}_\uparrow$ can be decomposed into the spatial and spin parts,

$$\begin{aligned}&\left\langle \tilde{\Psi}^{(S')}_{r'\{n'\}S'} \middle| \hat{U}_\uparrow \middle| \tilde{\Psi}^{(S)}_{r\{n\}S} \right\rangle \\ &\quad = (f_S f_{S'})^{-1/2} \sum_{t,t',i} \left\langle \tilde{\Phi}^{(S')}_{t'r'\{n'\}} \middle| U(\mathbf{r}_i) \middle| \tilde{\Phi}^{(S)}_{tr\{n\}} \right\rangle \left\langle \Xi^{(S')}_{t'S'} \middle| \uparrow(i) \right\rangle \\ &\qquad \times \left\langle \uparrow(i) \middle| \Xi^{(S)}_{tS} \right\rangle. \end{aligned} \tag{27}$$

The spatial matrix elements are given by Eq. (25). The spin matrix elements include projections of the spin wave functions (14)

$$\left\langle \uparrow(i) \middle| \Xi^{(S)}_{tS} \right\rangle = C_{SS} \sum_{\mathcal{P}} D^{[\lambda]}_{t[0]}(\mathcal{P}) \sum_{l=1}^{\lambda_1} \delta_{i\mathcal{P}l} \times \prod_{j\neq l}^{\lambda_1} |\uparrow(\mathcal{P}j)\rangle \prod_{j=\lambda_1+1}^{N} |\downarrow(\mathcal{P}j)\rangle.$$

Substituting $\mathcal{P} = \mathcal{Q}\mathcal{P}_{l\lambda_1}$ we get

$$\left\langle \uparrow(i) \middle| \Xi^{(S)}_{tS} \right\rangle = C_{SS} \sum_{\mathcal{Q}} \sum_{l=1}^{\lambda_1} D^{[\lambda]}_{t[0]}(\mathcal{Q}\mathcal{P}_{l\lambda_1}) \delta_{i\mathcal{Q}\lambda_1} \times \prod_{j=1}^{\lambda_1-1} |\uparrow(\mathcal{Q}j)\rangle \prod_{j=\lambda_1+1}^{N} |\downarrow(\mathcal{Q}j)\rangle.$$

The permutation $\mathcal{P}_{l\lambda_1}$ permute symbols in the first row of the Young tableau [0]. Therefore, $D^{[\lambda]}_{t[0]}(\mathcal{Q}\mathcal{P}_{l\lambda_1}) = D^{[\lambda]}_{t[0]}(\mathcal{Q})$ [see Eq. (8)], the summand in the equation above is independent of l, and the projection can be expressed as

$$\left\langle \uparrow(i) \middle| \Xi^{(S)}_{tS} \right\rangle = \lambda_1 C_{SS} \sum_{\mathcal{Q}} D^{[\lambda]}_{t[0]}(\mathcal{Q}) \delta_{i\mathcal{Q}\lambda_1} \times \prod_{j=1}^{\lambda_1-1} |\uparrow(\mathcal{Q}j)\rangle \prod_{j=\lambda_1+1}^{N} |\downarrow(\mathcal{Q}j)\rangle.$$

The projection involved into matrix elements of $\hat{U}_{-1}$ is evaluated in the same way,

$$\left\langle \downarrow(i) \middle| \Xi^{(S)}_{tS} \right\rangle = \lambda_2 C_{SS} \sum_{\mathcal{Q}} D^{[\lambda]}_{t[0]}(\mathcal{Q}) \delta_{i\mathcal{Q}(\lambda_1+1)} \times \prod_{j=1}^{\lambda_1} |\uparrow(\mathcal{Q}j)\rangle \prod_{j=\lambda_1+2}^{N} |\downarrow(\mathcal{Q}j)\rangle.$$

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

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

the permutations $\mathcal{R}$ and $\mathcal{Q}$ can be different by permutations $\mathcal{P}'$ of the first $\lambda_1 - 1$ 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], we have $D^{[\lambda]}_{t'[0]}(\mathcal{R}) = D^{[\lambda]}_{t'[0]}(\mathcal{Q})$ [see Eq. (8)]. Since the numbers of permutations $\mathcal{P}'$ and $\mathcal{P}''$ are $(\lambda_1 - 1)!$ and $\lambda_2!$, respectively, the spin matrix elements take the form

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

Let us substitute this equation and (25) into (27), perform the summation over t and t' using Eq. (6), and substitute $\mathcal{P} = \mathcal{Q}^{-1}\mathcal{R}^{-1}$, $j = \mathcal{R}i$. Then the Kronecker symbol leads to $\mathcal{P}j = \mathcal{Q}^{-1}i = \lambda_1$, and we get

$$\left\langle \tilde{\Psi}^{(S)}_{r'\{n'\}S} \middle| \hat{U}_\uparrow \middle| \tilde{\Psi}^{(S)}_{r\{n\}S} \right\rangle = \lambda_1!\lambda_2!\lambda_1 C^2_{SS} \sum_{\mathcal{P}} D^{[\lambda]}_{[0]r'}(\mathcal{P}) D^{[\lambda]}_{[0]r}(\mathcal{P}) \times \sum_{j=1}^{N} \delta_{\lambda_1\mathcal{P}j} \langle n'_j|U|n_j\rangle \prod_{j'\neq j} \delta_{n'_{j'},n_{j'}}. \tag{28}$$

The matrix element

$$\begin{aligned}&\left\langle \tilde{\Psi}^{(S-1)}_{r'\{n'\}S-1} \middle| \hat{U}_{-1} \middle| \tilde{\Psi}^{(S)}_{r\{n\}S} \right\rangle \\ &\quad = \frac{1}{\sqrt{2}} \lambda_1!\lambda_2!(\lambda_2+1) C_{SS} C_{S-1S-1} \sum_{\mathcal{P}} D^{[\lambda']}_{[0]r'}(\mathcal{P}) D^{[\lambda]}_{[0]r}(\mathcal{P}) \\ &\qquad \times \sum_{j=1}^{N} \delta_{\lambda_1\mathcal{P}j} \langle n'_j|U|n_j\rangle \prod_{j'\neq j} \delta_{n'_{j'},n_{j'}}, \end{aligned} \tag{29}$$

where $\lambda' = [\lambda_1 - 1, \lambda_2 + 1]$, is calculated in a similar way.

The explicit expressions (28) and (29) are rather complicated as they include Young orthogonal matrices and summation over all permutations. The next section provides expressions for sums of the matrix elements and their squared moduli, which are much simpler.

C. Sum rules

The sum of diagonal in total spin S and r matrix elements can be written out as

$$\sum_r \langle \tilde{\Psi}^{(S)}_{r'\{n'\}S} | \hat{U}_a | \tilde{\Psi}^{(S)}_{r\{n\}S} \rangle = Y^{(S)}[\hat{U}_a] \frac{f_S}{N} \sum_{j=1}^{N} \langle n'_j | U | n_j \rangle \prod_{j' \neq j} \delta_{n'_{j'}, n_{j'}}. \quad (30a)$$

The universal factors $Y^{(S)}$ are independent of the matrix elements $\langle n'_j | U | n_j \rangle$. For $\hat{U}_\uparrow$, the factor $Y^{(S)}[\hat{U}_\uparrow]$ can be derived from (28) using the equalities $\sum_r D^{[\lambda]}_{[0]r}(\mathcal{P}) D^{[\lambda]}_{[0]r}(\mathcal{P}) = D^{[\lambda]}_{[0][0]}(\mathcal{E}) = 1$ [obtained with (6) and (7)] and $\sum_{\mathcal{P}} \delta_{\lambda_1 \mathcal{P} j} = (N-1)!$, as

$$Y^{(S)}[\hat{U}_\uparrow] = \frac{N}{2} + S. \quad (30b)$$

It is equal to the number of the spin-up atoms. For the spherical vector component $\hat{U}_0$, the factor $Y^{(S)}[\hat{U}_0]$ is obtained using Eq. (22),

$$Y^{(S)}[\hat{U}_0] = S. \quad (30c)$$

Equation (26) leads to

$$Y^{(S)}[\hat{U}] = N. \quad (30d)$$

The sum of squared moduli of the matrix elements (28) and (29) can be expressed, using Eqs. (4) and (15), as

$$\sum_{r,r'} \left| \langle \tilde{\Psi}^{(S)}_{r'\{n'\}S} | \hat{U}_\uparrow | \tilde{\Psi}^{(S)}_{r\{n\}S} \rangle \right|^2 = \left(\frac{\lambda_1 f_S}{N!} \right)^2 \sum_{jj'} \Sigma^{(S,S)}_{jj'} \langle n'_j | U | n_j \rangle \langle n_{j'} | U | n'_{j'} \rangle \times \prod_{j'' \neq j} \delta_{n'_{j''}, n_{j''}} \prod_{j''' \neq j'} \delta_{n'_{j'''}, n_{j'''}}, \quad (31)$$

$$\sum_{r,r'} \left| \langle \tilde{\Psi}^{(S-1)}_{r'\{n'\}S-1} | \hat{U}_{-1} | \tilde{\Psi}^{(S)}_{r\{n\}S} \rangle \right|^2 = \frac{\lambda_1(\lambda_2+1) f_S f_{S-1}}{2(N!)^2} \sum_{jj'} \Sigma^{(S-1,S)}_{jj'} \langle n'_j | U | n_j \rangle \langle n_{j'} | U | n'_{j'} \rangle \times \prod_{j'' \neq j} \delta_{n'_{j''}, n_{j''}} \prod_{j''' \neq j'} \delta_{n'_{j'''}, n_{j'''}}, \quad (32)$$

where

$$\Sigma^{(S',S)}_{jj'} = \sum_{r,r'} \sum_{\mathcal{P}} D^{[\lambda']}_{[0]r'}(\mathcal{P}) D^{[\lambda]}_{[0]r}(\mathcal{P}) \delta_{\lambda_1 \mathcal{P} j} \times \sum_{\mathcal{Q}} D^{[\lambda']}_{[0]r'}(\mathcal{Q}) D^{[\lambda]}_{[0]r}(\mathcal{Q}) \delta_{\lambda_1 \mathcal{Q} j'}. \quad (33)$$

These sums are calculated in the Appendix. It is shown that

$$\Sigma^{(S,S)}_{jj} = \frac{N!(N-1)!}{f_S \lambda_1^2} \left[\lambda_1 - \frac{\lambda_2}{\lambda_1 - \lambda_2 + 2} \right], \quad (34)$$

$$\Sigma^{(S-1,S)}_{jj} = \frac{N!(N-1)!}{f_S \lambda_1} \quad (35)$$

are independent of j, and

$$\Sigma^{(S',S)}_{jj'} = \frac{N!(N-2)!}{f_S} \delta_{SS'} - \frac{1}{N-1} \Sigma^{(S',S)}_{jj} \quad (36)$$

for any $j' \neq j$.

If the sets of spatial quantum numbers $\{n\}$ and $\{n'\}$ are different, the product of Kronecker symbols in (31) and (32) does not vanish only if $j = j'$. Then the sum of squared moduli of the matrix elements can be written out as

$$\sum_{r,r'} \left| \langle \tilde{\Psi}^{(S')}_{r'\{n'\}S} | \hat{U}_a | \tilde{\Psi}^{(S)}_{r\{n\}S} \rangle \right|^2 = Y^{(S,1)}[\hat{U}_a, \hat{U}_a] \frac{f_{S'}}{N} \sum_{j=1}^{N} |\langle n'_j | U | n_j \rangle|^2 \prod_{j' \neq j} \delta_{n'_{j'}, n_{j'}}, \quad (37a)$$

where $S' \leqslant S$ and the difference $S - S'$ is unambiguously determined by the operator $\hat{U}_a$. Each term in the sum here changes one spatial quantum number, conserving other ones. If $U(\mathbf{r}) = \text{const}$, the sums vanish since $\langle \varphi_{n'} | U | \varphi_n \rangle = U \langle \varphi_{n'} | \varphi_n \rangle = 0$ for $n \neq n'$. The universal factors $Y^{(S,1)}[\hat{U}_a, \hat{U}_a]$, which are independent of the matrix elements $\langle n'_j | U | n_j \rangle$, are expressed in terms of $\Sigma^{(S',S)}_{jj}$. Then Eqs. (34) and (35) lead to

$$Y^{(S,1)}[\hat{U}_\uparrow, \hat{U}_\uparrow] = \frac{N}{2} + S - \frac{N - 2S}{4(S+1)}, \quad (37b)$$

$$Y^{(S,1)}[\hat{U}_{-1}, \hat{U}_{-1}] = \frac{N - 2S + 2}{4}, \quad (37c)$$

and Eq. (26) gives

$$Y^{(S,1)}[\hat{U}, \hat{U}] = N.$$

The factor $Y^{(S,1)}[\hat{U}_0, \hat{U}_0]$ for the spherical vector component $\hat{U}_0$ is obtained using (22). Since the matrix elements of $\hat{U}$ are diagonal in r [see Eq. (26)], one gets

$$Y^{(S,1)}[\hat{U}_0, \hat{U}_0] = \frac{S(N+2)}{4(S+1)}. \quad (37d)$$

For transitions conserving the spatial quantum numbers, $\{n'\} = \{n\}$ and the Kronecker symbols in (31) and (32) are equal to 1 for any j and j'. Then sums of squared moduli of the matrix elements can be represented as

$$\sum_{r,r'} \left| \langle \tilde{\Psi}^{(S')}_{r'\{n\}S'} | \hat{U}_a | \tilde{\Psi}^{(S)}_{r\{n\}S} \rangle \right|^2 = f_{S'} \left[Y^{(S,0)}_0[\hat{U}_a, \hat{U}_a] \langle U \rangle^2 + Y^{(S,0)}_1[\hat{U}_a, \hat{U}_a] \langle \Delta U \rangle^2 \right], \quad (38a)$$

where

$$\langle U \rangle = \frac{1}{N} \sum_{j=1}^{N} \langle n_j | U | n_j \rangle$$

is the average matrix element and

$$\langle \Delta U \rangle = \left[\frac{1}{N} \sum_{j=1}^{N} (\langle n_j | U | n_j \rangle - \langle U \rangle)^2 \right]^{1/2}$$

is the average deviation of the matrix elements of $U(\mathbf{r})$. The universal factors $Y^{(S,0)}_0[\hat{U}_a, \hat{U}_a]$ and $Y^{(S,0)}_1[\hat{U}_a, \hat{U}_a]$ are

independent of the matrix elements $\langle n_j|U|n_j\rangle$. Equations (34)–(36) lead to

$$Y_0^{(S,0)}[\hat{U}_a,\hat{U}_a] = \left(Y^{(S)}[\hat{U}_a]\right)^2 \tag{38b}$$

[where we define $Y^{(S)}[\hat{U}_{-1}] = 0$, in addition to Eq. (30)], and

$$Y_1^{(S,0)}[\hat{U}_{-1},\hat{U}_{-1}] = \frac{N(N-2S+2)}{4(N-1)}, \tag{38c}$$

$$Y_1^{(S,0)}[\hat{U}_{\uparrow},\hat{U}_{\uparrow}] = Y_1^{(S,0)}[\hat{U}_0,\hat{U}_0] = \frac{S(N-2S)(N+2S+2)}{4(S+1)(N-1)}. \tag{38d}$$

If $U(\mathbf{r}) = \text{const}$, $\Delta U = 0$, and, therefore, $\sum_{r,r'} |\langle\tilde{\Psi}^{(S-1)}_{r'\{n\}S-1}|\hat{U}_{-1}|\tilde{\Psi}^{(S)}_{r\{n\}S}\rangle|^2 = 0$. Indeed, in this case, the spatial matrix elements (25) are equal to zero due to the orthogonality of the spatial wave functions with different spins.

Thus, sums of matrix elements and their squared moduli are expressed in terms of universal factors, which are independent of the spatial orbitals and details of the external fields, and sums of one-body matrix elements (or their squared moduli), which are independent of many-body spins. The sum rules, combined with the spin-projection dependence (23), provide information on each matrix element for an one-body spin-dependent interaction with an external field.

IV. SUM RULES FOR TWO-BODY SPIN-INDEPENDENT INTERACTIONS

The permutation-invariant interaction between particles is given by

$$\hat{V} = \sum_{j\neq j'} V(\mathbf{r}_j - \mathbf{r}_{j'}). \tag{39}$$

Without loss of generality, we can restrict consideration to even potential functions, $V(\mathbf{r}) = V(-\mathbf{r})$, since their odd parts are canceled. Matrix elements of this interaction can be evaluated for general spin wave functions. Due to the orthogonality of the spin wave functions (10), the matrix elements are diagonal in spin quantum numbers and can be reduced to the matrix elements between spatial wave functions,

$$\left\langle\tilde{\Psi}^{(S')}_{r'\{n'\}l'}\middle|\hat{V}\middle|\tilde{\Psi}^{(S)}_{r\{n\}l}\right\rangle = \delta_{SS'}\delta_{ll'}\frac{2}{f_S}\sum_t\sum_{i<i'}\left\langle\tilde{\Phi}^{(S)}_{tr'\{n'\}}\middle|V(\mathbf{r}_i-\mathbf{r}_{i'})\middle|\tilde{\Phi}^{(S)}_{tr\{n\}}\right\rangle \tag{40}$$

(this reduction is used in spin-free quantum chemistry [6,7]). Then, using (11), (39), and the property (7) of the Young orthogonal matrices, the spatial matrix elements can be expressed as

$$\left\langle\tilde{\Phi}^{(S)}_{tr'\{n'\}}\middle|V(\mathbf{r}_i-\mathbf{r}_{i'})\middle|\tilde{\Phi}^{(S)}_{tr\{n\}}\right\rangle = \frac{f_S}{N!}\sum_{\mathcal{R},\mathcal{Q}}\text{sgn}(\mathcal{Q})D^{[\lambda]}_{r't}(\mathcal{Q})\text{sgn}(\mathcal{R})D^{[\lambda]}_{rt}(\mathcal{R}) \times\int d^Dr_i d^Dr_{i'}\varphi^*_{n'_{\mathcal{Q}i}}(\mathbf{r}_i)\varphi^*_{n'_{\mathcal{Q}i'}}(\mathbf{r}_{i'})V(\mathbf{r}_i-\mathbf{r}_{i'})\varphi_{n_{\mathcal{R}i}}(\mathbf{r}_i)\varphi_{n_{\mathcal{R}i'}}(\mathbf{r}_{i'})\prod_{i'\neq i''\neq i}\delta_{n'_{\mathcal{Q}i''},n_{\mathcal{R}i''}}. \tag{41}$$

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 $\mathcal{Q} = \mathcal{R}\mathcal{P}_{ii'}$. Then substitution of (41) into (40), using (6) and (7), leads to

$$\left\langle\tilde{\Psi}^{(S')}_{r'\{n'\}l'}\middle|\hat{V}\middle|\tilde{\Psi}^{(S)}_{r\{n\}l}\right\rangle = 2\delta_{SS'}\delta_{ll'}\frac{1}{N!}\sum_{\mathcal{R}}\sum_{i<i'}\prod_{\mathcal{R}i'\neq j''\neq\mathcal{R}i}\delta_{n'_{j''},n_{j''}}\left[\delta_{r'r}\langle n'_{\mathcal{R}i}n'_{\mathcal{R}i'}|V|n_{\mathcal{R}i}n_{\mathcal{R}i'}\rangle + \text{sgn}(\mathcal{P}_{ii'})D^{[\lambda]}_{r'r}(\mathcal{R}\mathcal{P}_{ii'}\mathcal{R}^{-1})\langle n'_{\mathcal{R}i'}n'_{\mathcal{R}i}|V|n_{\mathcal{R}i}n_{\mathcal{R}i'}\rangle\right], \tag{42}$$

where $\langle n'_1n'_2|V|n_1n_2\rangle = \int d^Dr_1d^Dr_2\varphi^*_{n'_1}(\mathbf{r}_1)\varphi^*_{n'_2}(\mathbf{r}_2)V(\mathbf{r}_1-\mathbf{r}_2)\varphi_{n_1}(\mathbf{r}_1)\varphi_{n_2}(\mathbf{r}_2)$.

Taking into account that

$$\mathcal{P}\mathcal{P}_{ii'}\mathcal{P}^{-1} = \mathcal{P}_{\mathcal{P}i\mathcal{P}i'} \tag{43}$$

(see [7]) and substituting $\mathcal{R}i = j$, one finally gets

$$\left\langle\tilde{\Psi}^{(S')}_{r'\{n'\}l'}\middle|\hat{V}\middle|\tilde{\Psi}^{(S)}_{r\{n\}l}\right\rangle = 2\delta_{SS'}\delta_{ll'}\sum_{j<j'}\prod_{j'\neq j''\neq j}\delta_{n'_{j''},n_{j''}}\left[\delta_{r'r}\langle n'_jn'_{j'}|V|n_jn_{j'}\rangle + \text{sgn}(\mathcal{P}_{jj'})D^{[\lambda]}_{r'r}(\mathcal{P}_{jj'})\langle n'_{j'}n'_j|V|n_jn_{j'}\rangle\right]. \tag{44}$$

It is a special case of the matrix elements obtained by Heitler [8] and Kaplan [6].

The sum of diagonal elements of the representation matrix, the character

$$\chi_S(\mathcal{C}) \equiv \sum_r D^{[\lambda]}_{rr}(\mathcal{P}),$$

is the same for all permutations $\mathcal{P}$, which form the class of conjugate elements $\mathcal{C}$ [4–7]. Table II presents the characters for the classes appearing here. (Supplemental material for [17] contains a code based on the explicit expressions [34] for the characters.) The conjugated classes of the symmetric group $\mathcal{S}_N$ are characterized by the cyclic structure of the permutations. All permutations in the class $\mathcal{C} = \{N^{\nu_N}\ldots 2^{\nu_2}\}$ have ν_l cycles of length l. This class notation omits l^{ν_l} if $\nu_l = 0$ and the

TABLE II. Characters $\chi_S(\mathcal{C})$ of the classes $\mathcal{C}$ of conjugate elements of the symmetric group $\mathcal{S}_N$ of permutations of N symbols in the irreducible representations, corresponding to the spin S. The characters are calculated with the Frobenius formula [7,33] and scaled to the representation dimension f_S.

$\mathcal{C}$	$\chi_S(\mathcal{C})/f_S$
$\{2\}$	$\frac{4S^2+N^2+4S-4N}{2N(N-1)}$
$\{3\}$	$\frac{12S^2+N^2+12S-10N}{4N(N-1)}$
$\{4\}$	$\frac{N^4-24N^3+4N^2(6S^2+6S+29)-16N(10S^2+10S+9)+16S(S+1)(S^2+S+12)}{8N(N-1)(N-2)(N-3)}$
$\{2^2\}$	$\frac{N^4-12N^3+8N^2(S^2+S+7)+8N(10S^2+10S+9)+16S(S+1)(S^2+S+6)}{4N(N-1)(N-2)(N-3)}$

number of cycles of the length one, i.e., the number of symbols which are not affected by the permutations in the class. This number is determined by the condition $\sum_{l=1}^{N} l\nu_l = N$. Permutations of two symbols form the class $\{2\}$. This leads to the sum of diagonal in r matrix elements

$$\sum_r \langle \tilde{\Psi}^{(S)}_{r\{n'\}l} | \hat{V} | \tilde{\Psi}^{(S)}_{r\{n\}l} \rangle = 2 \sum_{j<j'} \left[f_S \langle n'_j n'_{j'} | V | n_j n_{j'} \rangle \pm \chi_S(\{2\}) \langle n'_{j'} n'_j | V | n_j n_{j'} \rangle \right] \times \prod_{j' \neq j'' \neq j} \delta_{n'_{j''}, n_{j''}}, \tag{45a}$$

where the sign + or − is taken for bosons or fermions, respectively. Similar expressions have been obtained for the total energy [8] and arbitrary observables [17]. If $\{n'\} = \{n\}$, the Kronecker symbols are equal to 1 for any j and j' and the sum can be transformed to the form

$$\sum_r \langle \tilde{\Psi}^{(S)}_{r\{n\}l} | \hat{V} | \tilde{\Psi}^{(S)}_{r\{n\}l} \rangle = N(N-1) f_S \left(\langle V \rangle_{\rm dir} \pm \frac{\chi_S(\{2\})}{f_S} \langle V \rangle_{\rm ex} \right). \tag{45b}$$

Here and above, the dependence on many-body states is given by universal functions f_S and $\chi_S(\{2\})$, which are independent of the matrix elements $\langle n'_1 n'_2 | V | n_1 n_2 \rangle$, while the average matrix elements

$$\langle V \rangle_{\rm dir} = \frac{2}{N(N-1)} \sum_{j<j'} \langle n_j n_{j'} | V | n_j n_{j'} \rangle, \qquad \langle V \rangle_{\rm ex} = \frac{2}{N(N-1)} \sum_{j<j'} \langle n_{j'} n_j | V | n_j n_{j'} \rangle \tag{46}$$

of the direct and exchange interactions, respectively, are independent of the many-body states.

Calculating the sum of squared moduli of the matrix elements (44), one can see that if the sets of spatial quantum numbers $\{n\}$ and $\{n'\}$ are different by two elements, the product of Kronecker symbols in the product of the matrix elements does not vanish only if the pair j, j' is the same in both matrix elements. Then the sum can be expressed as

$$\sum_{r,r'} \left| \langle \tilde{\Psi}^{(S)}_{r'\{n'\}l} | \hat{V} | \tilde{\Psi}^{(S)}_{r\{n\}l} \rangle \right|^2 = 4 f_S \sum_{j<j'} \prod_{j' \neq j'' \neq j} \delta_{n'_{j''}, n_{j''}} \Big[|\langle n'_j n'_{j'} | V | n_j n_{j'} \rangle|^2 + |\langle n'_{j'} n'_j | V | n_j n_{j'} \rangle|^2 \pm 2 \frac{\chi_S(\{2\})}{f_S} \mathrm{Re}(\langle n'_j n'_{j'} | V | n_j n_{j'} \rangle \langle n'_{j'} n'_j | V | n_j n_{j'} \rangle^*) \Big]. \tag{47a}$$

Here the equality $\sum_{rr'} D^{[\lambda]}_{r'r}(\mathcal{P}_{jj'}) D^{[\lambda]}_{r'r}(\mathcal{P}_{jj'}) = \sum_r D^{[\lambda]}_{rr}(\mathcal{E}) = f_S$ was used. Each term in the sum above changes two of the spatial quantum numbers, conserving other ones. The case of a single changed quantum number will be considered elsewhere.

For transitions conserving the spatial quantum numbers, $\{n'\} = \{n\}$ and the Kronecker symbols in (44) are equal to 1 for any j and j'. Then

$$\sum_{r,r'} \left| \langle \tilde{\Psi}^{(S)}_{r'\{n\}l} | \hat{V} | \tilde{\Psi}^{(S)}_{r\{n\}l} \rangle \right|^2 = \Big[f_S N^2 (N-1)^2 \langle V \rangle^2_{\rm dir} \pm 2\chi_S(\{2\}) N^2 (N-1)^2 \langle V \rangle_{\rm dir} \langle V \rangle_{\rm ex} + \sum_{j_1 \neq j'_1} \sum_{j_2 \neq j'_2} \sum_r D^{[\lambda]}_{rr}(\mathcal{P}_{j_1 j'_1} \mathcal{P}_{j_2 j'_2}) \langle n_{j'_1} n_{j_1} | V | n_{j_1} n_{j'_1} \rangle \langle n_{j'_2} n_{j_2} | V | n_{j_2} n_{j'_2} \rangle \Big]$$

The trace of the Young matrix can be transformed in the following way (since $j_1 \neq j'_1$ and $j_2 \neq j'_2$):

$$\sum_r D^{[\lambda]}_{rr}(\mathcal{P}_{j_1 j'_1} \mathcal{P}_{j_2 j'_2}) = \chi_S(\{2^2\}) + (\delta_{j_1 j_2} + \delta_{j_1 j'_2} + \delta_{j'_1 j_2} + \delta_{j'_1 j'_2})[\chi_S(\{3\}) - \chi_S(\{2^2\})] + (\delta_{j_1 j_2} \delta_{j'_1 j'_2} + \delta_{j_1 j'_2} \delta_{j'_1 j_2})[f_S - 2\chi_S(\{3\}) + \chi_S(\{2^2\})],$$

since $\mathcal{P}_{j_1 j'_1} \mathcal{P}_{j_1 j'_2} \in \{3\}$ for $j'_1 \neq j'_2$, $\mathcal{P}_{j_1 j'_1} \mathcal{P}_{j_1 j'_1} = \mathcal{E}$, and $\chi_S(\mathcal{E}) = f_S$. Here and in what follows, $\chi_S(\{3\})$ and $\chi_S(\{2^2\})$ have to be equated to zero at $N < 3$ and $N < 4$, respectively, when the corresponding permutations do not exist. Using the identity $2f_S + 4(N-2)\chi_S(\{3\}) + (N-2)(N-3)\chi_S(\{2^2\}) = N(N-1)\chi^2_S(\{2\})/f_S$ (it can be directly proved with the characters in Table II), the sum of squared moduli of the matrix elements can be represented as

$$\sum_{r,r'} \left| \langle \tilde{\Psi}^{(S)}_{r'\{n\}l} | \hat{V} | \tilde{\Psi}^{(S)}_{r\{n\}l} \rangle \right|^2 = f_S \left(Y^{(S,0)}_1 [\hat{V}, \hat{V}] \langle \Delta_1 V \rangle^2 + Y^{(S,0)}_2 [\hat{V}, \hat{V}] \langle \Delta_2 V \rangle^2 \right) + \frac{1}{f_S} \left(\sum_r \langle \tilde{\Psi}^{(S)}_{r\{n\}l} | \hat{V} | \tilde{\Psi}^{(S)}_{r\{n\}l} \rangle \right)^2 \tag{47b}$$

with the universal factors

$$Y_1^{(S,0)}[\hat{V},\hat{V}] = 4N(N-1)^2\frac{\chi_S(\{3\})-\chi_S(\{2^2\})}{f_S}, \quad Y_2^{(S,0)}[\hat{V},\hat{V}] = 2N(N-1)\left(1-\frac{2\chi_S(\{3\})-\chi_S(\{2^2\})}{f_S}\right). \tag{47c}$$

Here

$$\langle\Delta_1 V\rangle^2 = \frac{1}{N}\sum_{j=1}^{N}\left(\frac{1}{N-1}\sum_{j'\neq j}\langle n_{j'}n_j|V|n_jn_{j'}\rangle - \langle V\rangle_{\rm ex}\right)^2,$$
$$\langle\Delta_2 V\rangle^2 = \frac{2}{N(N-1)}\sum_{j<j'}(\langle n_{j'}n_j|V|n_jn_{j'}\rangle - \langle V\rangle_{\rm ex})^2 \tag{48}$$

measure the average deviation of the exchange matrix elements.

Thus, sums of matrix elements and their squared moduli are expressed in terms of universal factors, which are independent of the spatial orbitals and interaction potentials, and sums of two-body matrix elements (or their squared moduli), which are independent of the many-body spins. The universal factors are expressed in terms of characters of irreducible representations of the symmetric group. The characters are functions of the total spin and the number of particles.

V. MULTIPLET ENERGIES FOR WEAKLY INTERACTING GASES

As an example of applications of the sum rules, consider splitting of degenerate energy levels due to weak two-body spin-independent interactions. The Hamiltonian of the system is a sum of one-body Hamiltonians $\hat{H}_0(j)$ of noninteracting particles and two-body interactions (39),

$$\hat{H}_{\rm spat} = \sum_{j=1}^{N}\hat{H}_0(j) + \hat{V}. \tag{49}$$

The interactions split energies of the degenerate states (13). In the zero order of the degenerate perturbation theory [3], the eigenenergies E_{Sn} (counted from the multiplet-independent energy of noninteracting particles $\sum_{j=1}^{N}\varepsilon_{n_j}$) are determined by the secular equation

$$\sum_{r'}V_{rr'}^{(S)}A_{nr'}^{(S)} = E_{Sn}A_{nr}^{(S)}, \tag{50}$$

where $A_{nr}^{(S)}$ are the expansion coefficients of the wave function (16) in terms of the wave functions of noninteracting particles (17),

$$\Psi_{nS_z}^{(S)} = \sum_{r}A_{nr}^{(S)}\tilde{\Psi}_{r\{n\}S_z}^{(S)} \tag{51}$$

and the matrix elements of the spin-independent two-body interaction (44)

$$V_{rr'}^{(S)} = \langle\tilde{\Psi}_{r'\{n\}S_z}^{(S)}|\hat{V}|\tilde{\Psi}_{r\{n\}S_z}^{(S)}\rangle$$

do not couple states with different spins.

Consider at first the case when the matrix elements $V_{\rm dir} = \langle n_1n_2|\hat{V}|n_1n_2\rangle$ and $V_{\rm ex} = \langle n_1n_2|\hat{V}|n_2n_1\rangle$ are independent of the spatial quantum numbers. E.g., this can take place in the case of zero-range interactions $V(\mathbf{r}) = V\delta(\mathbf{r})$, if the spatial orbitals have a form of plane waves. In this case, the summation over $\mathcal{R}$ in the matrix element (42) for $\{n\} = \{n'\}$ can be performed using Eqs. (6), (7), and the orthogonality relation (5) in the following way [5]:

$$\sum_{\mathcal{R}}D_{r'r}^{[\lambda]}(\mathcal{R}\mathcal{P}_{ii'}\mathcal{R}^{-1}) = \sum_{t,t'}D_{t't}^{[\lambda]}(\mathcal{P}_{ii'})\sum_{\mathcal{R}}D_{r't'}^{[\lambda]}(\mathcal{R})D_{rt}^{[\lambda]}(\mathcal{R})$$
$$= \frac{N!}{f_S}\delta_{r'r}\chi_S(\{2\}).$$

Then the matrix elements become diagonal in r,

$$V_{rr'}^{(S)} = \delta_{rr'}N(N-1)\left(V_{\rm dir}\pm\frac{\chi_S(\{2\})}{f_S}V_{\rm ex}\right),$$

where the character $\chi_S(\{2\})$ is given in Table II and the sign + or − is taken for bosons or fermions, respectively. The secular equation (50) is then satisfied by the eigenvectors $A_{nr}^{(S)} = \delta_{nr}$ and eigenvalues $E_{Sn} = V_{rr}^{(S)}$. Then all eigenstates with the given spin remain degenerate in energy. However, states with different total spins have different energies.

In the general case, when the matrix elements of $\hat{V}$ depend on the spatial quantum numbers, the energies E_{Sn} cannot be expressed in a simple form. However, using the equivalence of the sum of matrix eigenvalues to its trace and the sum of matrix elements (45b), the average multiplet energy can be expressed as

$$\bar{E}_S \equiv \frac{1}{f_S}\sum_{n}E_{Sn} = \frac{1}{f_S}\sum_{r}V_{rr}$$
$$= N(N-1)\left(\langle V\rangle_{\rm dir}\pm\frac{\chi_S(\{2\})}{f_S}\langle V\rangle_{\rm ex}\right), \tag{52}$$

where the average interactions $\langle V\rangle_{\rm dir}$ and $\langle V\rangle_{\rm ex}$ are defined by (46). (Here and below, the summation over n means the summation over states of interacting particles in a given spin multiplet with a given set $\{n\}$.) It is a particular case of the general expression obtained by Heitler [8]. The average energies are plotted in Fig. 1.

As the interaction lifts degeneracy of states with different total spins, transformation of the set of states with defined total spins to the set of states with given spin projections of particles becomes impossible. Then the former set remains the only valid set of eigenstates of interacting particles.

For fermions, the average multiplet energy decreases with S. The Lieb-Mattis theorem [23] predicts opposite dependence. However, this theorem is formulated for the lowest-energy states with given S, which can involve different sets of $\{n\}$ and have multiple occupation of spatial orbitals. In contrast, the average energies (52) are obtained for the fixed set of $\{n\}$ and single occupations.

The root-mean-square energy width of the spin-S multiplet $\langle\Delta E_S\rangle$ is defined by

$$\langle\Delta E_S\rangle^2 \equiv \frac{1}{f_S}\sum_{n}(E_{Sn}-\bar{E}_S)^2 = \frac{1}{f_S}\sum_{n}E_{Sn}^2 - \bar{E}_S^2.$$

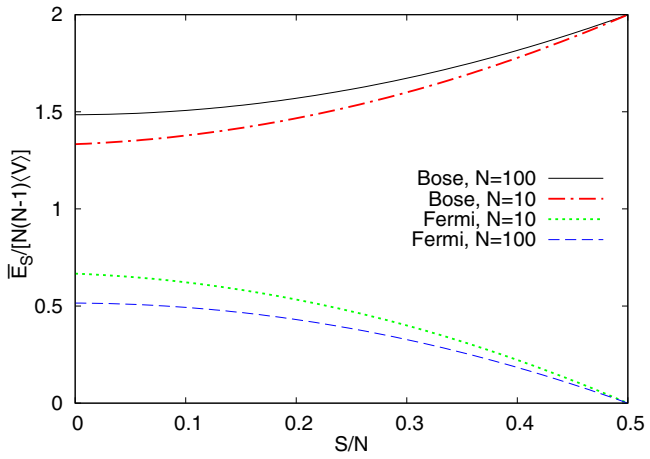

FIG. 1. (Color online) Scaled average multiplet energies $\bar{E}_S$ as functions of the multiplet spin S for N bosons or fermions. The energies are calculated with Eq. (52) and scaled characters from Table II, assuming $\langle V\rangle_{\rm dir} = \langle V\rangle_{\rm ex} = \langle V\rangle$.

Due to orthogonality of the expansion coefficients, the secular equation (50) can be rewritten in the form $E_{Sn}\delta_{n'n} = \sum_{rr'} A^*_{nr} V_{rr'} A_{n'r'}$, leading to

$$\frac{1}{f_S}\sum_{n,n'} |E_{Sn}\delta_{n'n}|^2 = \frac{1}{f_S}\sum_{r,r'} V^*_{rr'} V_{r'r}.$$

Then Eq. (47b) gives us

$$\langle \Delta E_S\rangle^2 = Y_1^{(S,0)}[\hat{V},\hat{V}]\langle\Delta_1 V\rangle^2 + Y_2^{(S,0)}[\hat{V},\hat{V}]\langle\Delta_2 V\rangle^2, \quad (53)$$

where the universal factors $Y_1^{(S,0)}[\hat{V},\hat{V}]$ and $Y_2^{(S,0)}[\hat{V},\hat{V}]$ are expressed in terms of the representation characters by Eq. (47c), and the matrix element deviations $\langle\Delta_1 V\rangle$ and $\langle\Delta_2 V\rangle$ are defined by Eq. (48). The multiplet energy widths are plotted in Fig. 2. If the matrix elements of $\hat{V}$ are independent of the spatial quantum numbers, $\langle\Delta_1 V\rangle = \langle\Delta_2 V\rangle = 0$ and, therefore, $\langle\Delta E_S\rangle = 0$, in agreement with the above-mentioned degeneracy of states with given S in this case. The energy width is determined by characters, which were identified by Dirac [35] as constants of motions, corresponding to

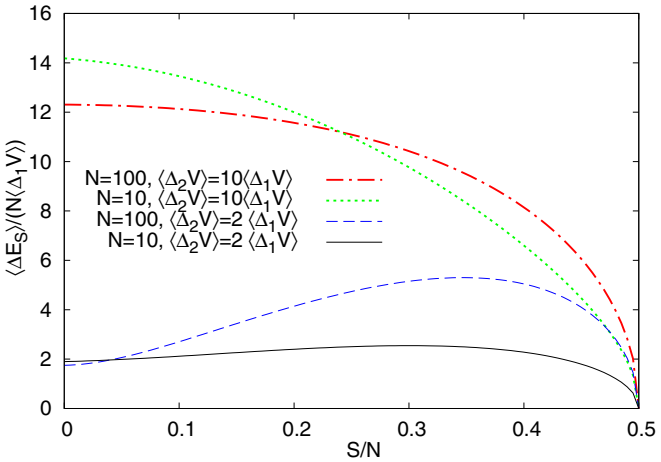

FIG. 2. (Color online) Scaled root-mean-square energy widths of multiplets as functions of the multiplet spin S for N particles, calculated with Eq. (53).

permutation symmetry, according to generalized Noether' s theorem. Therefore, the energy width can be considered as a conserved physical observable, related to this symmetry, as well as the average multiplet energy and correlations [17].

Using characters from Table II, the exact expression can be approximated at $N \gg 1$ by

$$\langle\Delta E_S\rangle^2 \approx \frac{N^2-4S^2}{2N^2} V_{1D}^2 [2N(4S^2-3N)\langle\Delta_1 V\rangle^2 + (3N^2-4S^2)\langle\Delta_2 V\rangle^2].$$

Consider now external fields described by one-body interactions. Matrix elements of a spin-independent field (26) are independent of r and spin quantum numbers. Therefore, this field leads to the same shift for all states, corresponding to the given set of spatial quantum numbers $\{n\}$. In the first order of the perturbation theory, this shift will be $\sum_{j=1}^N \langle n_j|U|n_j\rangle$. Even a strong spin-independent field leads to the same shift of all states, as it can be incorporated into the Hamiltonian of noninteracting particles. Then, the Schrödinger equation (12) will contain $\hat{H}_0(j) + U(\mathbf{r}_j)$. This leads to different one-body eigenfunctions $\varphi_n(\mathbf{r})$ and eigenvalues ε_n, but does not change the form of many-body wave functions.

Spin-dependent spatially homogeneous interactions [Eqs. (21) and (22) with $U = \text{const}$] commute with the spatial Hamiltonian of interacting particles (49). Since the spin wave functions (14) are eigenfunctions of such interactions, the eigenfunctions $\Psi^{(S)}_{nS_z}$ of $\hat{H}_{\rm spat}$ will be eigenfunctions of the Hamiltonian $\hat{H}_{\rm spat} + \hat{U}_0$. The energy shift of the states of noninteracting particles due to the field $\hat{U}_0$ is equal to the matrix element $\langle\tilde{\Psi}^{(S)}_{r'\{n\}S_z}|\hat{U}_0|\tilde{\Psi}^{(S)}_{r\{n\}S_z}\rangle = \delta_{r'r}S_z U$. It is determined by Eqs. (22), (23), (26), and (28), taking into account that $\langle n'|U|n\rangle = U\delta_{nn'}$. The energy shift of the states of interacting particles (51) will be the same, as $\langle\Psi^{(S)}_{nS_z}|\hat{U}_0|\Psi^{(S)}_{nS_z}\rangle = S_z U\sum_r A^*_{nr}A_{nr} = S_z U$.

The spin-independent inhomogeneous and spin-dependent homogeneous fields, considered above, are consistent with the separation (1) of the spin and spatial Hamiltonians. If the external field depends both on spins and coordinates, this separation is violated, invalidating the use of collective spin and spatial wave functions for noninteracting particles. Nevertheless, these wave functions remain applicable to interacting particles whenever the external field is weak enough, and the energy shift can be estimated in the first order of the perturbation theory. The average shift is calculated using orthogonality of the coefficients A_{nr}, Eqs. (23) and (30) in the following way:

$$\begin{aligned}
&\frac{1}{f_S}\sum_n \left\langle\Psi^{(S)}_{nS_z}\middle|\hat{U}_0\middle|\Psi^{(S)}_{nS_z}\right\rangle \\
&= \frac{1}{f_S}\sum_n A^*_{nr'}A_{nr}\left\langle\tilde{\Psi}^{(S)}_{r'\{n\}S_z}\middle|\hat{U}_0\middle|\tilde{\Psi}^{(S)}_{r\{n\}S_z}\right\rangle \\
&= X^{(S,S,1)}_{S_z 0} Y^{(S)}[\hat{U}_0]\frac{1}{N}\sum_{j=1}^N \langle n_j|U|n_j\rangle \\
&= \frac{S_z}{N}\sum_{j=1}^N \langle n_j|U|n_j\rangle. \qquad (54)
\end{aligned}$$

VI. CONCLUSIONS

The symmetric group methods allow us to evaluate the matrix elements of spin-dependent external fields (21) and spin-independent two-body interactions (39) in the basis with collective spin and spatial wave functions (2). These matrix elements agree to the selection rules [17]. For the matrix elements of spin-dependent external fields, explicit dependence on the total spin projection (23) is obtained using the Wigner-Eckart theorem. Analytical expressions are derived for sums of these matrix elements (30) and their squared moduli [Eqs. (37) and (38)] over irreducible representations for both spin-conserving and spin-changing transitions. Dependence on the many-body states in these sums is given by the $3j$ Wigner symbols and the universal factors $Y^{(S)}$, $Y^{(S,1)}$, $Y_0^{(S,0)}$, and $Y_1^{(S,0)}$. These factors are independent of details of one-body Hamiltonians and external fields and are expressed in a rather simple form in terms of the total spin and number of particles. For spin-independent two-body interactions, the sums of matrix elements (45) and their squared moduli (47) depend on the many-body states only through the representation characters, which were identified by Dirac [35] as constants of motions, corresponding to permutation symmetry. The sum rules can be applied to the evaluation of energy-level shifts (54), splitting of states with different total spins (52), and spin-multiplet energy widths (53). Other possible applications of the sum rules include estimates of the spin-multiplet depletion rates due to spin-dependent perturbations, as well as the population transfer rates between spin-multiplets using the spatially homogeneous spin-changing and spatially inhomogeneous spin-conserving pulses [17].

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APPENDIX: CALCULATION OF THE SUMS (33)

Using the relations (6) and (7) and substitution $\mathcal{R} = \mathcal{Q}\mathcal{P}^{-1}$, the sum (33) can be represented in the following form:

$$\Sigma_{jj'}^{(S',S)} = \sum_{\mathcal{R}} D_{[0][0]}^{[\lambda']}(\mathcal{R}) D_{[0][0]}^{[\lambda]}(\mathcal{R}) \sum_{\mathcal{P}} \delta_{\lambda_1,\mathcal{P}j}\delta_{\lambda_1,\mathcal{R}\mathcal{P}j'},$$

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

For $j = j'$, there are $(N-1)!$ permutations $\mathcal{P}$ such that $\mathcal{P}j = \lambda_1$. Then

$$\Sigma_{jj}^{(S',S)} = (N-1)! \sum_{\mathcal{R}} D_{[0][0]}^{[\lambda']}(\mathcal{R}) D_{[0][0]}^{[\lambda]}(\mathcal{R}) \delta_{\lambda_1,\mathcal{R}\lambda_1} \tag{A1}$$

is independent of j.

For $j \neq j'$, we have

$$\begin{aligned}\sum_{\mathcal{P}} \delta_{\lambda_1,\mathcal{P}j}\delta_{\lambda_1,\mathcal{R}\mathcal{P}j'} &= \sum_{l\neq\lambda_1} \delta_{\lambda_1,\mathcal{R}l} \sum_{\mathcal{P}} \delta_{l,\mathcal{P}j'}\delta_{\lambda_1,\mathcal{P}j} \\ &= (N-2)! \sum_{l} \delta_{\lambda_1,\mathcal{R}l}\left(1-\delta_{\lambda_1 l}\right) \\ &= (N-2)!\left(1-\delta_{\lambda_1,\mathcal{R}\lambda_1}\right).\end{aligned}$$

Then

$$\begin{aligned}\Sigma_{jj'}^{(S',S)} &= \sum_{\mathcal{R}} D_{[0][0]}^{[\lambda']}(\mathcal{R}) D_{[0][0]}^{[\lambda]}(\mathcal{R}) (N-2)!\left(1-\delta_{\lambda_1,\mathcal{R}\lambda_1}\right) \\ &= \frac{N!(N-2)!}{f_S}\delta_{\lambda\lambda'} - \frac{1}{N-1}\Sigma_{jj}^{(S',S)},\end{aligned} \tag{A2}$$

where the last transformation uses Eqs. (5) and (A1). The last expression in (A2) is independent of j and j' and equivalent to (36).

The Young orthogonal matrix elements in (A1) have been calculated by Goddard [36] in the following way. Each permutation $\mathcal{R}$ can be represented as

$$\mathcal{R} = \prod_{k=1}^{n_{\rm ex}} \mathcal{P}_{i'_k i''_k} \mathcal{P}' \mathcal{P}'',$$

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 [36]

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

Due to the Kronecker symbols in Eq. (A1), the permutations $\mathcal{P}'$ do not affect λ_1 and $i'_k \leqslant \lambda_1 - 1$. 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 $\binom{\lambda_1-1}{n_{\rm ex}}$ and $\binom{\lambda_2}{n_{\rm ex}}$, respectively. Then for $S = S'$ Eq. (A1) can be transformed as follows:

$$\begin{aligned}\Sigma_{jj}^{(S,S)} &= (N-1)! \sum_{n_{\rm ex}=0}^{\lambda_2} (\lambda_1-1)!\lambda_2! \binom{\lambda_1-1}{n_{\rm ex}}\binom{\lambda_2}{n_{\rm ex}}\binom{\lambda_1}{n_{\rm ex}}^{-2} \\ &= \frac{(N-1)!(\lambda_2!)^2}{\lambda_1^2} \sum_{n_{\rm ex}=0}^{\lambda_2} \frac{(\lambda_1-n_{\rm ex})!}{(\lambda_2-n_{\rm ex})!}(\lambda_1-n_{\rm ex}).\end{aligned}$$

The sum over $n_{\rm ex}$ can be calculated, leading to (34).

If $S' = S-1$ we have

$$\begin{aligned}\Sigma_{jj}^{(S-1,S)} &= (N-1)! \sum_{n_{\rm ex}=0}^{\lambda_2} (\lambda_1-1)!\lambda_2! \binom{\lambda_1-1}{n_{\rm ex}} \\ &\quad\times \binom{\lambda_2}{n_{\rm ex}}\binom{\lambda_1}{n_{\rm ex}}^{-1}\binom{\lambda_1-1}{n_{\rm ex}}^{-1} \\ &= \frac{(N-1)!(\lambda_2!)^2}{\lambda_1} \sum_{n_{\rm ex}=0}^{\lambda_2} \frac{(\lambda_1-n_{\rm ex})!}{(\lambda_2-n_{\rm ex})!},\end{aligned}$$

giving (35).

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