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

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Many-body eigenstates of spin-1/2 particles with defined total spins contain spin and spatial wavefunctions belonging to multidimensional irreducible representations of the symmetric group, unless the total spin has the maximal allowed value. Matrix elements in the basis of such eigenstates are analyzed for spin-dependent interactions with external fields and spin-independent ones between the particles. Analytical expressions are obtained for sums of the matrix elements and sums of their squared modules. The sum rules are applied to perturbative analysis of energy spectra.

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INTRODUCTION

Calculations of quantum-mechanical system properties require matrix elements between its states. For complex systems, even calculation of the matrix elements can constitute a complicated problem. However, in certain cases, sum rules (see [1]) can be derived from general principles, providing analytical expressions for sums of matrix elements or their products. Sum rules are widely used in atomic, 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 which 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. States of such systems can be described in two ways (see [2]). In the first one, each particle is characterized by its spin and coordinate, and the total wavefunction is symmetrized for bosons or antisymmetrized for fermions over permutations of all particles. In this approach, each spin state constitutes an independent component. The second approach is based on collective spin and spatial wavefunctions. These wavefunctions depend on spins or coordinates, respectively, of all particles and form representations of the symmetric group (see [3–6]). 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 wavefunctions belong to multidimensional, non-Abelian, representations of the symmetric group (see [3–6]), beyond the conventional paradigm of symmetric-antisymmetric functions. The symmetric or antisymmetric total wavefunction is represented as a sum of products of the spin and spatial wavefunctions. This way is used in spin-free quantum chemistry [5, 6] and spinor quantum gases [7–10]. Such gases are intensively studied starting from the first experimental [11, 12] and theoretical [13, 14] works (see book [15], reviews [16, 17] and references therein). \( SU(M) \)-symmetric gases, introduced in [9, 18, 19] and recently observed in [20, 21], are described in terms of the collective spin and spatial wavefunctions too [9]. The symmetric group was also applied to spinor gases in [22–26].

In the case of non-interacting particles in spin-independent potentials, all states with the given set of spatial quantum numbers are energy-degenerate and the two kinds of wavefunctions are applicable, being related by a linear transformation. However, spin-independent interactions of particles lift the degeneracy of states with different total spins, as has been already shown by Heitler [27], and the wavefunctions with defined individual spins become inapplicable.

The sum of matrix elements of spin-independent inter-particle interactions has been obtained by Heitler [27]. The present paper provides the sums of squared modules of these matrix elements, as well as sums of matrix elements and their squared modules for spin-dependent external fields. Such fields can be used for transfer of population between states with different total spins, as described in [10].

The representations of spinor, spatial, and total wavefunctions are given in Sec. I. Section II contains derivation of the sum rules. The sum rules are applied to description of the shift and splitting of energy levels in Sec. III.

I. THE HAMILTONIAN AND WAVEFUNCTIONS

Consider a system of \( N \) particles with the Hamiltonian

\[
\hat{H} = \hat{H}_{\text{spat}} + \hat{H}_{\text{spin}}
\]  

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

The total wavefunction is expressed in the form

\[
\psi_{nl}^{(S)} = \int S^{1/2} \sum_{t} \phi_{tn}^{(S)} \Xi_{tl}^{(S)}.
\]
It is a sum of products of spatial $\Phi_{tn}^{(S)}$ and spin $\Xi_{tl}^{(S)}$ functions, which form irreducible representations of the symmetric group $S_N$ of $N$-symbol permutations,[3–6]. This means that a permutation $P$ of the particles transforms each function to a linear combination of functions in the same representation,

$$\mathcal{P}\Phi_{tn}^{(S)} = \text{sgn}(P) \sum_t D^{[\lambda]}_t(P)\Phi_{tn}^{(S)}$$

$$\mathcal{P}\Xi_{tl}^{(S)} = \sum_t D^{[\lambda]}_t(P)\Xi_{tl}^{(S)}$$

Here the factor $\text{sgn}(P)$ is the permutation parity for fermions and $\text{sgn}(P) = 1$ for bosons. This factor provides the proper permutation symmetry of the total wavefunction

$$\mathcal{P}\Psi_{nl}^{(S)} = \text{sgn}(P)\Psi_{nl}^{(S)}$$

The matrices of the Young orthogonal representation [3–6] $D^{[\lambda]}_t(P)$ of the symmetric group $S_N$ 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 $\lambda$. The dimension of the representation is equal to the number of different tableaux,

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

If $S = N/2$, $f_S = 1$, $D^{[\lambda]}_t(P) = 1$, and the functions $\Phi_{tn}^{(S)}$ and $\Xi_{tl}^{(S)}$ remain unchanged on permutations of particles or change their sign ($\Phi_{tn}^{(S)}$ for fermions). Otherwise, the functions belong to multidimensional, non-Abelian irreducible representations of the symmetric group.

The Young orthogonal matrices obey the orthogonality relation[5, 6]

$$\sum_t D^{[\lambda]}_{t'}(P)D^{[\lambda]}_t(P) = \frac{N!}{f_S} \delta_{tt'}\delta_{rr'}\delta_{\lambda\lambda'},$$

the general relation for representation matrices

$$\sum_t D^{[\lambda]}_{t'}(P)D^{[\lambda]}_t(Q) = D^{[\lambda]}_{t'}(PQ),$$

and the relation for orthogonal matrices

$$D^{[\lambda]}_t(P^{-1}) = D^{[\lambda]}_t(P).$$

The spatial and spin wavefunctions form orthonormal basis sets,

$$\langle \Phi_{tn'}^{(S')}|\Phi_{tn}^{(S)} \rangle = \delta_{S'S}\delta_{tt'}\delta_{nn'}$$

$$\langle \Xi_{tl'}^{(S')}|\Xi_{tl}^{(S)} \rangle = \delta_{S'S}\delta_{tt'}\delta_{ll'}$$

$$\Phi_{tn}^{(S)} = f_S^{-1/2} \sum_t \Phi_{tn}^{(S)} \Xi_{tl}^{(S)}.$$  (15)

The spatial functions of non-interacting particles are expressed as [5, 6]

$$\Phi_{tr\{n\}}^{(S)} = \left(\frac{f_S}{N!}\right)^{1/2} \sum_P \text{sgn}(P)D^{[\lambda]}_t(P)\prod_{j=1}^N \varphi_n(r_P)$$

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

$$\hat{H}_0(j)\varphi_n(r_j) = \varepsilon_n\varphi_n(r_j),$$

where $r_j$ is the $D$-dimensional coordinate of $j$th 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. All quantum numbers $n_j$ in the set $\{n\}$ are supposed to be different. The functions (10) satisfy the Schrödinger equation

$$\sum_{j=1}^N \hat{H}_0(j)\Phi_{tr\{n\}}^{(S)} = \sum_{j=1}^N \varepsilon_{n_j}\Phi_{tr\{n\}}^{(S)}.$$  (11)

Their eigenenergies are independent of $r$. Therefore, there are $f_S$ degenerate states of non-interacting particles for each set $\{n\}$. Equation (2) gives us the total wavefunctions of non-interacting particles

$$\Psi_{tr\{n\}}^{(S)} = f_S^{-1/2} \sum_t \Phi_{tr\{n\}}^{(S)} \Xi_{tl}^{(S)}.$$  (12)

In the absence of interactions between spins, the spin wavefunction are eigenfunctions of the total spin projection operator $S_z$ and can be expressed as

$$\Xi_{tl}^{(S)} = C_{SS_z} \sum_P D^{[\lambda]}_t(P) \prod_{j=1}^{N_2+S_2} | \uparrow(P_j) \rangle \prod_{j=N_2+S_2+1}^N | \downarrow(P_j) \rangle.$$  (13)

In the case of the spin wavefunction, each of two spin states, $|\uparrow\rangle$ and $|\downarrow\rangle$, has to be occupied by several particles, if $N > 2$. This leads to the normalization factor [28]

$$C_{SS_z} = \frac{1}{(N/2+S_2)!(N/2-S_2)!} \sqrt{\frac{(2S+1)(S+S_2)!}{(N/2+S+1)(2S)!(S-S_2)!}},$$

unlike the spatial wavefunction (10). Besides, the Young tableau $r$ can take now only one value $[0]$ — the Young tableau in which the symbols are arranged by rows in the sequence of natural numbers. As a result, only one representation is associated with given total spin $S$ and its projection $S_z$. The total wavefunction with the defined $S_z$ is then expressed as

$$\Phi_{tn}^{(S)} = f_S^{-1/2} \sum_t \Phi_{tn}^{(S)} \Xi_{tl}^{(S)}.$$  (15)
In combination with the spatial wavefunction (10), the spin wavefunctions lead to the total wavefunctions of non-interacting particles,

\[
\tilde{\Psi}(S)_{r(\{n\})S_z} = f_S^{-1/2} \sum_i \tilde{\Phi}(S)_{tr(\{n\})} \Xi(S).
\] (16)

There are \(f_S\) wavefunctions, labeled by the Young tableau \(r\), having the total spin \(S\) and the set of spatial quantum numbers \(\{n\}\). Then the total number of wavefunctions with the given total spin projection \(S_z\) will be \(\sum_{S_z} f_S = N!/[(N/2+S_z)!(N/2-S_z)!]\). It is the number of distinct choices of \(N/2 + S_z\) particles with spin up and is then equal to the number of states with given spin projection of each of \(N\) particles. Then the set of degenerate states (16) can be unitarily transformed to the set of states with the given spin projections of particles. Such transformation becomes impossible for interacting particles, when the energy degeneracy is lifted, as shown by Heitler [27] and will be discussed in Sec. III.

II. SUM RULES FOR THE MATRIX ELEMENTS

A. One-body interactions

1. The spin-projection dependence

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

\[
\hat{U} = \sum_j U(r_j)
\] (17)

and three spherical vector components

\[
\hat{U}_0 = \sum_j U(r_j)\hat{s}_z(j), \quad \hat{U}_{\pm 1} = \mp \frac{1}{\sqrt{2}} \sum_j U(r_j)\hat{s}_{\pm}(j)
\] (18)

(see [29]). Here

\[
\hat{s}_z(j) = \frac{1}{2}(\uparrow(j)\downarrow(j) - \downarrow(j)\uparrow(j))
\]

is the \(z\)-component of the spin and

\[
\hat{s}_{+}(j) = \uparrow(j)\downarrow(j), \quad \hat{s}_{-}(j) = \downarrow(j)\uparrow(j)
\]

are the spin raising and lowering operators for \(j\)th 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 \(\hat{U}\),

\[
\hat{U}_+ = \sum_j U(r_j)\uparrow(j)\uparrow(j) = \hat{U}_0 + \frac{1}{2}\hat{U},
\]

\[
\hat{U}_- = \sum_j U(r_j)\downarrow(j)\downarrow(j) = -\hat{U}_0 + \frac{1}{2}\hat{U}.
\] (19)

| \(k\) | \(S - S_z\) | \(S\) | \(S'\) | \(S''\) | \(-S'' - S_z\) |
|-----|-----|-----|-----|-----|-----|
| 0   | \(\sqrt{S+1}\) \(\delta_{S,S'}\) \(\delta_{S_z,S_z'}\) \(|\tilde{\Psi}(S')_{r(\{n\})S_z}\rangle\langle\tilde{\Psi}(S)_{r(\{n\})0}\)| 1 |
| 1   | \(\sqrt{S+1}\) \(\frac{1}{\sqrt{2}}\) \(|\tilde{\Phi}(S)_{tr(\{n\})}\rangle\langle\tilde{\Phi}(S')_{tr(\{n\}')}\)| \(-S' - S_z\) |

Consider matrix elements of the spherical vector and scalar interactions between eigenfunctions (15) of \(\hat{S}_z\). Their dependence on \(\hat{S}_z\) follows from the Wigner-Eckart theorem (see [30]). The matrix elements of the spherical scalar (17) are diagonal in spins and independent of the spin projection,

\[
\langle\tilde{\Psi}(S')_{nS_z'}|\tilde{U}|\tilde{\Psi}(S)_{nS_z}\rangle = \delta_{SS'}\delta_{S_zS_z'}\langle\tilde{\Psi}(S')_{nS_z'}|\tilde{U}|\tilde{\Psi}(S)_{nS_z}\rangle.
\] (20)

The matrix elements of the spherical vector components (18) can be expressed in terms of the 3\(j\)-Wigner symbols as

\[
\langle\tilde{\Psi}(S')_{nS_z'}|\tilde{U}_{k}|\tilde{\Psi}(S)_{nS_z}\rangle = \delta_{S_zS_z'}\delta_{S_zS_z'}\langle\tilde{\Psi}(S')_{nS_z'}|\tilde{U}_{k}|\tilde{\Psi}(S)_{nS_z}\rangle = (-1)^{S'' - S_z} \left(\begin{array}{ccc} S & S' & 1 \\ S & -S' & -1 \\ S_z & S_z' & k \end{array}\right)^{-1}
\]

Here \(S' \leq S\) and the reduced matrix elements are expressed in terms of the matrix elements of \(\hat{U}_0\) for the maximal allowed spin projection. According to the properties of the 3\(j\)-Wigner symbols, the matrix elements (20) vanish if \(|S - S'| > 1\) (in agreement to the selection rules [10]). Values of non-vanishing coefficients, calculated with the 3\(j\)-Wigner symbols [2, 30], are presented in Tab. I. Hermitian conjugate of Eq. (20), together with relations \(\hat{U}_{-1} = -\hat{U}_{+1}^\dagger\) and \(\hat{U}_0 = \hat{U}_0^\dagger\), give us the matrix elements for \(S' = S + 1\).

2. Sum rules

Matrix elements of the spherical scalar (17) can be evaluated exactly for general spin wavefunctions. Due to the orthogonality of the spin wavefunctions (9), the matrix elements are diagonal in spin quantum numbers and can be reduced to the matrix elements between spatial wavefunctions,

\[
\langle\tilde{\Psi}(S')_{r(\{n'\})l'}|\tilde{U}|\tilde{\Psi}(S)_{r(\{n\})l}\rangle = \delta_{SS'}\delta_{ll'} \frac{1}{f_S} f_S \sum_i \langle\tilde{\Phi}(S)_{tr(\{n\})}\rangle\langle\tilde{\Phi}(S')_{tr(\{n'\})}\rangle.
\] (21)

Let us calculate the spatial matrix element for the general case, \(S \neq S'\), having in mind further analysis of spherical

\[
\langle\tilde{\Psi}(S)_{r(\{n\})l}|\tilde{U}|\tilde{\Psi}(S')_{r(\{n'\})l'}\rangle
\]

\[
\langle\tilde{\Psi}(S)_{r(\{n\})l}|\tilde{U}|\tilde{\Psi}(S')_{r(\{n'\})l'}\rangle
\]
vectors. Equations (10) and (7) lead to

\[
\langle \hat{\Phi}^{(S')}_{t',r'}|U(r)|\hat{\Phi}^{(S)}_{t,r} \rangle = \frac{\sqrt{fs}}{N!} \sum_{R,Q} sgn(Q) D^{[\lambda]}_{t',r'}(Q) \times sgn(R) D^{[\lambda]}_{t,r}(R) \langle \varphi_{n',q'}|U(r)|\varphi_{n,q} \rangle \prod_{j \neq i} \delta_{n'_j,q'_j - n_j}. \quad (22)
\]

The Kronecker \(\delta\)-symbols appear here due to the orthogonality of the spatial orbitals \(\varphi_n\) and the absence of equal quantum numbers in each of the sets \(\{n\}\) and \(\{n'\}\). In each term in the sum over \(j\), all but one spatial quantum numbers remain unchanged. 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 \(Q = R\), and therefore,

\[
\langle \hat{\Psi}^{(S')}_{t',r'}|U|\hat{\Psi}^{(S)}_{t,r} \rangle = \frac{\sqrt{fs}}{N} \sum_{R} D^{[\lambda]}_{t',r'}(R) D^{[\lambda]}_{t,r}(R) \times \langle \varphi_{n',q'}|U(r)|\varphi_{n,q} \rangle \prod_{j \neq i} \delta_{n'_j,q'_j - n_j}. \quad (23)
\]

Then, substituting this expression into (21), using (6), (7), and the property of representations \(D^{[\lambda]}_{t',r'}(E) = \delta_{t',r'}\), where \(E\) is the identity permutation, one finally gets

\[
\langle \hat{\Psi}^{(S')}_{t',r'}|U|\hat{\Psi}^{(S)}_{t,r} \rangle = \delta_{SS'} \delta_{ll'} \delta_{r,r'} \langle \{n'\}|U|\{n\} \rangle, \quad (23)
\]

where \(\langle \{n'\}|U|\{n\} \rangle = \sum_{j=1}^{N} (n'_j|U|n_j) \prod_{j \neq i} \delta_{n'_j,n_j} \) and \(\langle \{n'\}|U|n \rangle = \int d\varphi_{n'} \varphi_n (r) U(r) \varphi_n (r)\). It is a special case of the matrix elements obtained by Heitler [27] and Kaplan [5].

For the spherical vector interactions (18), the matrix elements cannot be represented in so simple a form. However, rather simple expressions can be derived for sums and sums of squared modules of the matrix elements between eigenfunctions of \(S_z\). It is enough to consider matrix elements of \(\hat{U}_1\) and the spin-up state interaction \(\hat{U}_1\) for the maximal allowed spin projection. \(S_z = S'\), \(S_z = S\), as (19) and the Wigner-Eckart theorem (20) relate to them each matrix element of each interaction. In the basis of the non-interacting particle wavefunctions (16), the matrix elements of \(\hat{U}_1\) can be decomposed into the spatial and spinor parts,

\[
\langle \hat{\Psi}^{(S')}_{t',r'}|\hat{U}_1|\hat{\Psi}^{(S)}_{t,r} \rangle = (fs)^{-1/2} \sum_{t',i} \langle \hat{\Phi}^{(S')}_{t',r'}|U(r)|\hat{\Phi}^{(S)}_{t,r} \rangle \langle \Xi^{(S')}_{t',r'}|U|\Xi^{(S)}_{t}\rangle \langle \uparrow (i)|\uparrow (i) \rangle \langle \uparrow (i)|\uparrow (i) \rangle. \quad (24)
\]

The spatial matrix elements are given by Eq. (22). The spinor matrices elements include projections of the spin wavefunction

\[
\langle \uparrow (i)|\Xi^{(S)}_{t}\rangle = C_{SS'} \sum_{\lambda} D^{[\lambda]}_{t} (P) \sum_{l=1}^{\lambda} \delta_{i+l} \times \prod_{j \neq l} \frac{1}{|\uparrow (Q_j)\rangle \langle \downarrow (Q_j)|} \quad (25)
\]

Substituting \(P = Q_\lambda_1\), we get

\[
\langle \uparrow (i)|\Xi^{(S)}_{t}\rangle = C_{SS'} \sum_{\lambda} D^{[\lambda]}_{t} (Q_\lambda_1) \delta_{i,Q_\lambda_1} \times \prod_{j=1}^{\lambda_1-1} \frac{1}{|\uparrow (Q_j)\rangle \langle \downarrow (Q_j)|}. \quad (25)
\]

The permutation \(P_\lambda\) permute symbols in the first row of the Young tableau \([0]\). Therefore, \(D^{[\lambda]}_{t} (P_\lambda) = \delta_{t}[0]\) (see [4-6]), \(D^{[\lambda]}_{t} (Q_\lambda_1) = \sum_{\lambda_1} D^{[\lambda]}_{t} (Q) D^{[\lambda]}_{t} (P_\lambda_1) = D^{[\lambda]}_{t} (Q)\), the summand in the equation above is independent of \(l\), and the projection can be expressed as

\[
\langle \uparrow (i)|\Xi^{(S)}_{t}\rangle = \lambda_1 C_{SS'} \sum_{\lambda} D^{[\lambda]}_{t} (Q) \delta_{i,Q_\lambda_1} \times \prod_{j=1}^{\lambda_1-1} \frac{1}{|\uparrow (Q_j)\rangle \langle \downarrow (Q_j)|}. \quad (25)
\]

The projection involved into matrix elements of \(\hat{U}_1\) is evaluated in the same way,

\[
\langle \downarrow (i)|\Xi^{(S)}_{t}\rangle = \lambda_2 C_{SS'} \sum_{\lambda} D^{[\lambda]}_{t} (Q) \delta_{i,Q_\lambda_1 + 1} \times \prod_{j=1}^{\lambda_1+1} \frac{1}{|\uparrow (Q_j)\rangle \langle \downarrow (Q_j)|}. \quad (25)
\]

The permutons \(\mathcal{R}\) and \(\mathcal{Q}\) can be different by permutations \(P'\) of the first \(\lambda_1 - 1\) symbols and \(P''\) of the last \(\lambda_2\) ones. As the permutations \(P'\) and \(P''\) do not permute symbols between rows in the Young tableau \([0]\),

\[
D^{[\lambda]}_{t} (P'P'') = \delta_{t}[0] \quad (25), \quad \text{and}
\]

\[
D^{[\lambda]}_{t} (Q_\lambda_1) = \sum_{\mathcal{R}} D^{[\lambda]}_{t} (P) D^{[\lambda]}_{t} (P'P'') = D^{[\lambda]}_{t} (P). \quad (25)
\]

Since the numbers of permutations \(P'\) and \(P''\) are \((\lambda_1 - 1)!\) and \(\lambda_2!\), respectively, the spinor matrix elements take the form,
The matrix element

\[
\langle \hat{U}_1 \Psi^{(S)}_{r' r(n') S \ldots 1} | U_1 \Psi^{(S)}_{r n S} \rangle = \frac{1}{\sqrt{2}} \lambda_1 ! \lambda_2 ! (\lambda_2 + 1) C \lambda_1 C \lambda_2 C \lambda_3 \cdots C \lambda_S \cdots C \lambda_{S-1} \cdots C \lambda_{S-1} !
\]

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

For \( \hat{U}_1 \) the sum of diagonal in \( r \) matrix elements can be calculated using the equalities \( \sum_r D^{[\lambda]}_{[0] r} (P) D^{[\lambda]}_{[0] r} (P) = D^{[\lambda]}_{[0] [0]} (E) = 1 \) [obtained with (6) and (7)] and \( \sum_P \delta_{\lambda r} = (\lambda - 1) ! \), as

\[
\sum_r \langle \hat{U}_1 \Psi^{(S)}_{r' r(n') S \ldots 1} | U_1 \Psi^{(S)}_{r n S} \rangle = f_S \left( \frac{1}{2} + \frac{N}{N - 1} \right) \{ n' \} | U \{ n \} \rangle.
\]

The sum of squared modules of the matrix elements (26) and (27) can be expressed, using Eqs. (4) and (14), as

\[
\sum r, r' | \langle \hat{U}_1 \psi^{(S)}_{r' r(n') S \ldots 1} | \Psi^{(S)}_{r n S} \rangle |^2 = \left( \frac{\lambda_1 f_S}{N!} \right)^2 \sum_{j'} \Sigma^{(S, S)}_{j j'} \langle n'_j | U | n_j \rangle \langle n'_j | U | n_j \rangle \prod_{j'' \neq j} \delta_{n''_j, n''_j} \prod_{j'''' \neq j'} \delta_{n''''_{j'}, n''''_{j'}}
\]

where

\[
\Sigma^{(S, S)}_{j j'} = \sum r, r' D^{[\lambda]}_{[0] r} (P) D^{[\lambda]}_{[0] R} (P) \delta_{\lambda r} \prod_P \sum_{j'' \neq j} \delta_{n''_j, n''_j} \prod_{j''' \neq j'} \delta_{n'''_{j'}, n'''_{j'}}
\]

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

\[
\Sigma^{(S, S)}_{j j'} = \sum_{R} D^{[\lambda]}_{[0] [0]} (R) D^{[\lambda]}_{[0] [0]} (R) \sum_{P} \delta_{\lambda r} \delta_{\lambda R} \prod_P \delta_{n''_j, n''_j} \prod_{j''' \neq j'} \delta_{n'''_{j'}, n'''_{j'}}
\]

These sums are calculated in Appendix. It is shown that

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

are independent of \( j \) and

\[
\Sigma^{(S', S)}_{j j'} = \frac{N!(N - 2)!}{f_S} \delta_{S S'} - \frac{1}{N - 1} \Sigma^{(S, S)}_{j j'}
\]

for any \( j' \neq j \).

If the sets of spatial quantum numbers \( \{ n \} \) and \( \{ n' \} \) are different, the product of Kronecker symbols in (29) and (30) does not zeroes only if \( j = j' \). Then Eqs. (32) and (33) lead to

\[
\sum_{r, r'} | \langle \hat{U}_1 \psi^{(S)}_{r' r(n') S \ldots 1} | \Psi^{(S)}_{r n S} \rangle |^2 = \sum_{j=1}^N \langle n'_j | U | n_j \rangle \prod_{j' \neq j} \delta_{n'_j, n_j} (34)
\]
\[
\sum_{r,r'} |\langle \tilde{\psi}_{r'}^{(S)} | \hat{U}_{-1} | \tilde{\psi}_{r}^{(S)} \rangle |^2 = f_{S-1} \frac{N - 2S + 2}{4N} - 2S + 2 \quad \sum_{j=1}^{N} |\langle n_j' | U | n_j \rangle |^2 \prod_{j' \neq j} \delta_{n_j', n_{j'}} \quad (36)
\]

Each term in the sums here changes one spatial quantum number, conserving other ones. If \( U(r) = \text{const.} \), the sums vanish since \( \langle \varphi_{n'} | U | \varphi_n \rangle = U \langle \varphi_{n'} | \varphi_n \rangle = 0 \) for \( n \neq n' \).

For transitions conserving the spatial quantum numbers, \( \{n'\} = \{n\} \) and the Kronecker symbols in (29) are equal to one for any \( j \) and \( j' \). Then for \( \hat{U}_{-1} \) Eq. (30) can be transformed, using Eqs. (33) and (34), to

\[
\sum_{r,r'} |\langle \tilde{\psi}_{r'}^{(S)} | \hat{U}_{-1} | \tilde{\psi}_{r}^{(S)} \rangle |^2 = f_{S-1} \frac{N(N - 2S + 2)}{4(N-1)} (\Delta U)^2
\]

where

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

is the average deviation of the matrix elements of \( U(r) \). If \( U(r) = \text{const.} \), \( \Delta U = 0 \), and the sum (37) vanishes. Indeed, in this case, the spatial matrix elements (22) are equal to zero due to the orthogonality of the spatial wavefunctions with different spins.

For \( \hat{U}_1 \) the similar derivation leads to

\[
\sum_{r,r'} |\langle \tilde{\psi}_{r'}^{(S)} | \hat{U}_1 | \tilde{\psi}_{r}^{(S)} \rangle |^2 = f_{S} \frac{S(N + 2S)(N + 2S + 2)}{4(S+1)(N-1)} (\Delta U)^2 + f_{S} \frac{N/2 + S}{2} \sum_{j=1}^{N} \langle n_j | U | n_j \rangle^2
\]

This sum does not vanish if \( U(r) = \text{const.} \).

Corresponding sums for \( \hat{U}_0 \) are obtained using (19). Since the matrix elements of \( \hat{U} \) are diagonal in \( r \) [see Eq. (23)], Eqs. (28), (35) and (38) lead to

\[
\sum_{r} |\langle \tilde{\psi}_{r}^{(S)} | \hat{U}_0 | \tilde{\psi}_{r}^{(S)} \rangle |^2 = f_{S} \frac{S(N + 2S)(N + 2S + 2)}{4(S+1)(N-1)} (\Delta U)^2 + f_{S} \frac{N/2 + S}{2} \sum_{j=1}^{N} \langle n_j | U | n_j \rangle^2
\]

B. Sum rules for two-body spin-independent interactions

The permutation-invariant interaction between particles is given by

\[
\hat{V} = \sum_{j \neq j'} V(r_j - r_{j'}). \quad (42)
\]

Without loss of generality, we can restrict consideration to even potential functions, \( V(r) = V(-r) \), since their odd parts are canceled. Matrix elements of this interaction can be evaluated for general spin wavefunctions. Due to the orthogonality of the spin wavefunctions (9), the matrix elements are diagonal in spin quantum numbers and can be reduced to the matrix elements between spatial wavefunctions,

\[
\langle \tilde{\psi}_{r'}^{(S')} | \hat{V} | \tilde{\psi}_{r}^{(S)} \rangle = \delta_{SS'} \delta_{ll'} \frac{2}{f_{S}} \sum_{i<d} \sum_{i'<d'} \langle \tilde{\psi}_{r'}^{(S')} | V(r_i - r_{i'}) | \tilde{\psi}_{r}^{(S)} \rangle.
\]

(43)
Then, using (10), (42), and the property (7) of the Young orthogonal matrices, the spatial matrix elements can be expressed as,

\[
\langle \tilde{\Psi}^{(S)}_{r'(n')} | V | \tilde{\Psi}^{(S)}_{r(n)} \rangle = \frac{f_S}{N_l} \sum_{R, \mathcal{Q}} \text{sgn}(\mathcal{Q}) D_{r|l}^{\mathcal{Q}}(\mathcal{Q}) \text{sgn}(\mathcal{R}) D_{r'|l'}^{\mathcal{R}}(\mathcal{R}) \\
\times \int d^D r_i d^D r_i' \varphi_{n_{\mathcal{Q}}'}^* (r_i) \varphi_{n_{\mathcal{R}}'}^* (r_i') V(r_i - r_i') \varphi_{n_{\mathcal{R}}}(r_i) \varphi_{n_{\mathcal{Q}}}(r_i') \prod_{i' \neq i'' \neq i} \delta_{n_{\mathcal{Q}}', n_{\mathcal{R}}', n_{\mathcal{R}}}. \tag{44}
\]

The Kronecker \(\delta\)-symbols appear here due to the orthogonality of the spatial orbitals \(\varphi_n\), and the absence of equal quantum numbers in each of the sets \(\{n\}\) and \(\{n'\}\). In each term in the sum over \(i\) and \(i'\) all but two spatial quantum numbers remain unchanged. 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 \(\mathcal{Q} = \mathcal{R} P_{i'}\). Then substitution of (44) into (43), using (6) and (7), leads to

\[
\langle \tilde{\Psi}^{(S')}_{r'(n')} | V | \tilde{\Psi}^{(S)}_{r(n)} \rangle = 2 \delta_{SS'} \delta_{ll'} \frac{1}{N_l} \sum_{R} \prod_{i < i' \neq j'' \neq i} \delta_{n_{i''}, n_{j''}} \\
\times \left[ \delta_{r-r'} \langle n_{R_i} n_{R_i'} \mid V \mid n_{R_i} n_{R_i'} \rangle + \text{sgn}(P_{i'}) D_{r|l'}^{\mathcal{R}}(\mathcal{R} P_{i'}^{-1}) \langle n_{R_i} n_{R_i'} \mid V \mid n_{R_i} n_{R_i'} \rangle \right], \tag{45}
\]

where \(\langle n_{i''} n_{i''} \mid V \mid n_{j''} n_{j''} \rangle = \int d^D r_i d^D r_2 \varphi_{n_{i''}}^* (r_i) \varphi_{n_{i''}}^* (r_2) V(r_i - r_2) \varphi_{n_{i''}} (r_i) \varphi_{n_{i''}} (r_2)\).

Taking into account that

\[PP_{i'} P_{i'}^{-1} = PP_{i'} P_{i'}\]

(see [6]) and substituting \(R_i = j\), one finally gets

\[
\langle \tilde{\Psi}^{(S')}_{r'(n')} | V | \tilde{\Psi}^{(S)}_{r(n)} \rangle = 2 \delta_{SS'} \delta_{ll'} \sum_{j < j' \neq j'' \neq j} \prod \delta_{n_{i''}, n_{j''}} \left[ \delta_{r-r'} \langle n_{j''} n_{j''} \mid V \mid n_{j''} n_{j''} \rangle + \text{sgn}(P_{j''}) D_{r|l'}^{\mathcal{R}}(P_{j''}) \langle n_{j''} n_{j''} \mid V \mid n_{j''} n_{j''} \rangle \right]. \tag{47}
\]

It is a special case of the matrix elements obtained by Heitler [27] and Kaplan [5].

**TABLE II.** Characters \(\chi_S(C)\) of the classes \(C\) of conjugate elements of the symmetric group \(S_N\) of permutations of \(N\) symbols in the irreducible representations, corresponding to the spin \(S\). The characters are calculated with the Frobenius formula [6, 31] and scaled to the representation dimension \(f_S\).

| \(C\) | \(\chi_S(C) / f_S\) |
|------|------------------|
| \{2\} | \(4^{N^2+4N^2-4N}\) |
| \{3\} | \(12^{N^2+4N^2-10N}\) |
| \{4\} | \(N^4 - 24N^2 + 4N(N^2 - 8 + 9 + 16N(S+1)S^2 + 12)\) |
| \{(2^3)\} | \(4^{N^2} - 8^N(S^2 + S^2 + S^2) + 8N(N^2 + 10N + 9) + 16N(S+1)S^2 + S^2 + 12\) |
| \{(2^3)\} | \(4^N(N-1)(N-2)(N-3)\) |

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

\[
\chi_S(C) = \sum_r D_{r|l}^{\mathcal{R}}(P),
\]

is the same for all permutations \(P\), which form the class of conjugate elements \(C\) [3–6]. Table II presents the characters for the classes appearing here. The conjugated classes of the symmetric group \(S_N\) are characterized by the cyclic structure of the permutations. All permutations in the class \(C = \{N^{nu} \ldots 2^nu\}\) have \(nu\) cycles of length \(l\). This class notation omits \(l^{nu}\) if \(nu = 0\) and the 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 \(\sum_{l=1}^{N} lu_l = N\). Transpositions form the class \(\{2\}\). This leads to the sum of diagonal in \(r\) matrix elements

\[
\sum_r \langle \tilde{\Psi}^{(S)}_{r(n')} | V | \tilde{\Psi}^{(S)}_{r(n)} \rangle = 2 \sum_{j < j'} f_S \langle n_{j'} n_{j'} | V | n_{j} n_{j} \rangle \pm \chi_S(\{2\}) \langle n_{j'} n_{j'} | V | n_{j} n_{j} \rangle \prod_{j' \neq j'' \neq j} \delta_{n_{j''}, n_{j''}}.
\]
where the sign $+$ or $-$ is taken for bosons or fermions, respectively. Similar expressions have been obtained for the total energy [27] and arbitrary observables [10]. If $\{n'\} = \{n\}$, the Kronecker symbols are equal to one for any $j$ and $j'$ and the sum can be transformed to the form

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

(48)

Here

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

(49)

are the average matrix elements of the direct and exchange interactions, respectively.

Calculating the sum of squared modules of the matrix elements (47), one can see that if the sets of spatial quantum numbers $\{n\}$ and $\{n'\}$ are different, the product of Kronecker symbols in the product of the matrix elements does not zeroes only if the pair $j, j'$ is the same in both matrix elements. Then the sum can be expressed as

$$
\sum_{r,r'} |(\tilde{\Psi}^{(S)}_{r\{n\}} | V | \tilde{\Psi}^{(S)}_{r\{n\}})|^2 = 4 f_S \sum_{j<j'} \prod_{j'
eq j} \delta_{n_{j'}, n_{j'}} \left[ |(n'_{j'} n_{j'}| V | n_{j} n_{j'})|^2 + |(n_{j'} n'_{j}| V | n_{j} n_{j'})|^2 \right]
$$

$$
\pm 2 \frac{\chi_S(\{2\})}{f_S} \text{Re} \left( \langle n'_{j'} n'_{j} | V | n_{j} n_{j'} \rangle \langle n_{j'} n'_{j} | V | n_{j} n_{j'} \rangle^* \right).
$$

Here the equality $\sum_{rr'} D_{rr'}^{[\lambda]} (\mathcal{P}_{jj'}) D_{rr'}^{[\lambda]} (\mathcal{P}_{jj'}) = \sum_r D_{rr}^{[\lambda]} (\mathcal{E}) = f_S$ was used. Each term in the sum above changes two of the spatial quantum numbers, conserving other ones.

For transitions conserving the spatial quantum numbers, $\{n'\} = \{n\}$ and the Kronecker symbols in (47) are equal to one for any $j$ and $j'$. Then

$$
\sum_{r,r'} |(\tilde{\Psi}^{(S)}_{r\{n\}} | V | \tilde{\Psi}^{(S)}_{r\{n\}})|^2 = f_S N^2 (N-1)^2 \langle V \rangle_{\text{dir}}^2 \pm 2 \chi_S(\{2\}) N^2 (N-1)^2 \langle V \rangle_{\text{dir}} \langle V \rangle_{\text{ex}}
$$

$$
+ \sum_{j_1 \neq j_1'} \sum_{j_2 \neq j_2'} \sum_r D_{rr}^{[\lambda]} (\mathcal{P}_{j_1 j_1'} \mathcal{P}_{j_2 j_2'}) \langle n_{j_1} n_{j_1'} | V | n_{j_1} n_{j_1'} \rangle \langle n_{j_2} n_{j_2'} | V | n_{j_2} n_{j_2'} \rangle
$$

The sum over $r$ of the Young matrices can be transformed in the following way (since $j_1 \neq j_1'$ and $j_2 \neq j_2'$)

$$
\sum_r D_{rr}^{[\lambda]} (\mathcal{P}_{j_1 j_1'} \mathcal{P}_{j_2 j_2'}) = \chi_S(\{2\}) + (\delta_{j_1 j_2} + \delta_{j_2 j_1} + \delta_{j_1' j_2} + \delta_{j_2' j_1'}) (\chi_S(\{3\}) - \chi_S(\{2\}))
$$

$$
+ (\delta_{j_1 j_2} \delta_{j_1' j_2'} + \delta_{j_1 j_2} \delta_{j_2' j_1'})(f_S - 2 \chi_S(\{3\}) + \chi_S(\{2\})),
$$

since $\mathcal{P}_{j_1 j_1'} \mathcal{P}_{j_2 j_2'} \in \{3\}$, $\mathcal{P}_{j_1 j_1'} \mathcal{P}_{j_2 j_2'} = \mathcal{E}$, and $\chi_S(\mathcal{E}) = f_S$. Using the identity $2 f_S + 4 (N-2) \chi_S(\{3\}) + (N-2)(N-3) \chi_S(\{2\}) = N(N-1) \chi_S^2(\{2\}) / f_S$ (it can be directly proved with the characters in Table II), the sum of squared modules of the matrix elements can be represented as

$$
\sum_{r,r'} |(\tilde{\Psi}^{(S)}_{r\{n\}} | V | \tilde{\Psi}^{(S)}_{r\{n\}})|^2 = 4 N(N-1)^2 \left[ \chi_S(\{3\}) - \chi_S(\{2\}) \right] \langle \Delta_1 V \rangle^2 + 2 N(N-1) \left[ f_S - 2 \chi_S(\{3\}) + \chi_S(\{2\}) \right] \langle \Delta_2 V \rangle^2
$$

$$
+ \frac{1}{f_S} \left( \sum_r |(\tilde{\Psi}^{(S)}_{r\{n\}} | V | \tilde{\Psi}^{(S)}_{r\{n\}})|^2 \right)^2.
$$

(50)

Here

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

$$
\langle \Delta_2 V \rangle^2 = \frac{2}{N(N-1)} \sum_{j<j'} \langle n_j n_{j'} | V | n_j n_{j'} \rangle - \langle \Delta_2 V \rangle_{\text{ex}}^2
$$

(51)

measure the average deviation of the exchange matrix elements.
III. 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 $H_0(j)$ of non-interacting particles and two-body interactions (42),

$$\hat{H}_{\text{spat}} = \sum_{j=1}^{N} \hat{H}_0(j) + \hat{V}$$  \hspace{1cm} (52)

The interactions split energies of the degenerate states (12). In the zero-order of the degenerate perturbation theory [2] the eigenenergies $E_{Sn}$ (counted from the multiplet-independent energy of non-interacting particles $\sum_{j=1}^{N} \varepsilon_{n_j}$) are determined by the secular equation

$$\sum_{r'} V_{rr'}^{(S)} A_{nr'}^{(S)} = E_{Sn} A_{nr}^{(S)}$$  \hspace{1cm} (53)

where $A_{nr}^{(S)}$ are the expansion coefficients of the wavefunction (15) in terms of the wavefunctions of non-interacting particles (16),

$$\Psi_{nS_z}^{(S)} = \sum_{r} A_{nr}^{(S)} \Psi_{r(n)S_z}^{(S)}$$  \hspace{1cm} (54)

and the matrix elements of the spin-independent two-body interaction (47)

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

do not couple states with different spins.

Consider at first the case when the matrix elements $\langle n_1' n_2' | V | n_1 n_2 \rangle$ of independent quantum numbers. E.g., this can take place if $V(r) = V \delta(r)$ and the spatial orbitals have a form of plane waves. In this case the summation over $R$ in the matrix element (45) can be performed using Eqs. (6), (7), and the orthogonality relation (5) in the following way [4]

$$\sum_{R} D_{r't}^{[A]} (R) P_{i'v} (R^{-1}) = \sum_{t,t'} D_{t't}^{[A]} (P_{i'v}) \sum_{R} D_{r't}^{[A]} (R) D_{r't}^{[A]} (R) \quad \frac{N!}{f_S} \delta_{r't} \chi_S(\{2\}).$$

Then the matrix elements become diagonal in $r$,

$$V_{rr'}^{(S)} = \delta_{rr'} N (N - 1) \left( V_{\text{dir}} \pm \frac{4S^2 + N^2 + 4S - 4N}{2N(N - 1)} V_{\text{ex}} \right)$$

where the average interactions $V_{\text{dir}}$ and $V_{\text{ex}}$ are defined by (49), the characters $\chi_S(\{2\})$ from Tab. II are used, and the sign $+$ or $-$ is taken for bosons or fermions, respectively. The secular equation (53) 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 $E_{Sn}$ can not 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 (48), the average multiplet energy can be expressed as

$$\bar{E}_S = \frac{1}{f_S} \sum_{n} E_{Sn} = \frac{1}{f_S} \sum_{n} V_{rr} = N(N - 1)$$

$$\times \left( V_{\text{dir}} \pm \frac{4S^2 + N^2 + 4S - 4N}{2N(N - 1)} V_{\text{ex}} \right).$$  \hspace{1cm} (55)

It is a particular case of the general expression obtained by Heitler [27]. (Here and below, the summation over $n$ means the summation over states of interacting particles in a given spin-multiplet with a given set $\{n\}$.)

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 eigenstates of interacting particles have to be represented as a sum of products of the collective spin and spatial wavefunctions.

The root-mean-square energy width of the spin-$S$ multiplet $\langle \Delta S^2 \rangle$ is defined by

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

Due to orthogonality of the expansion coefficients, the secular equation (53) can be rewritten in the form $E_{Sn} \delta_{n'n} = \sum_{r} A_{nr}^{*} V_{rr'} A_{n'r'}$, leading to

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

Then (50) gives us

$$\langle \Delta S^2 \rangle = 4N(N - 1)^2 \frac{\chi_S(\{3\}) - \chi_S(\{2^2\})}{f_S} \langle \Delta_1 V \rangle^2$$

$$+ 2N(N - 1) \left( 1 - \frac{2\chi_S(\{3\}) - \chi_S(\{2^2\})}{f_S} \right) \langle \Delta_2 V \rangle^2. $$

(56)

where $\langle \Delta_1 V \rangle$ and $\langle \Delta_2 V \rangle$ are defined by (51). 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, $\langle \Delta S^2 \rangle = 0$, 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 [32] as constants of motions, corresponding to 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 [10].

Using characters from Tab. 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 (23) 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 $|n \rangle$. In the first order of the perturbation theory, this shift will be $\sum_{j=1}^N \langle n_j | U | n_j \rangle$. Even strong spin-independent field leads to the same shift of all states, as it can be incorporated into the Hamiltonian of non-interacting particles. Then, the Schrödinger equation (11) will contain $\hat{H}_0(j) + U(r_j)$, leading to different one-body eigenfunctions $\varphi_n(r)$ and eigenvalues $\varepsilon_n$, but do not changing the form of many-body wavefunctions.

Spin-dependent spatially-homogeneous interactions [Eqs. (18) and (19) with $U = \text{const}$] commute with the spatial Hamiltonian of interacting particles (52). Since the spin wavefunctions (13) are eigenfunctions of such interactions, the eigenfunctions $\Psi_{nS_z}^{(S)}$ of $\hat{H}_{\text{spat}}$ will be eigenfunctions of the Hamiltonian $\hat{H}_{\text{spat}} + \hat{U}_0$. The energy shift of the states of non-interacting particles due to the field $\hat{U}_0$ is equal to the matrix element $\langle \Psi_{nS_z}^{(S)} | \hat{U}_0 | \Psi_{nS_z}^{(S)} \rangle = \delta_{r, r'} S_z U$. It is determined by Eqs. (19), (20), (23) and (26), taking into account that $(n' | U | n) = U \delta_{nn'}$. The energy shift of the states of interacting particles (54) will be the same, as $\langle \Psi_{nS_z}^{(S)} | \hat{U}_0 | \Psi_{nS_z}^{(S)} \rangle = S_z U \sum_r A_{n r} \Delta_{n r} = S_z U$.

The spin-independent inhomogeneous and spin-dependent homogeneous fields, considered above, are consistent with the separation (1) of the spinor 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 wavefunctions for non-interacting particles. Nevertheless, for interacting particles these wavefunctions remain applicable 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 $A_{n r}$ and Eqs. (20) and (39) in the following way,

$$\frac{1}{f S} \sum_n \langle \Psi_{r \{ n \} S_z}^{(S)} | \hat{U}_0 | \Psi_{nS_z}^{(S)} \rangle = \frac{1}{f S} \sum_n A_{n r} A_{n r} \langle \Psi_{r \{ n \} S_z}^{(S)} | \hat{U}_0 | \Psi_{r \{ n \} S_z}^{(S)} \rangle = \frac{S_z}{N} \sum_{j=1}^N \langle n_j | U | n_j \rangle.$$ 

CONCLUSIONS

The symmetric group methods allow to evaluate the matrix elements of spin-dependent external fields (18) and spin-independent two-body interactions (42) in the basis with collective spin and spatial wavefunctions (2). These matrix elements agree to the selection rules [10]. Explicit dependence on the total spin projection (20) is obtained using the Wigner-Eckart theorem. Rather simple analytical expressions are derived for sums of the matrix elements and their squares over irreducible representations for both spin-conserving and spin-changing transitions. The sums can be applied to the evaluation of energy-level shifts, including the splitting of states with different total spins (55) and spin-multiplet energy widths (56).

Appendix: Calculation of the sums (31)

The sum (31) is expressed as

$$\Sigma_{j j'}^{(S', S)} = \sum_{\mathcal{R}} D_{[\lambda]}^{[\lambda]} (\mathcal{R}) D_{[\lambda]}^{[\lambda]} (\mathcal{R}) \sum_{j \neq \lambda_1} \delta_{jj_1} \delta_{jj_1} \mathcal{R} \mathcal{P} j j'$$

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

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

is independent of $j$.

For $j \neq j'$ we have

$$\sum_{\mathcal{R}} \delta_{\lambda_1, \lambda_1} \mathcal{R} \mathcal{P} j j' = \sum_{i j \neq \lambda_1} \delta_{i j, \lambda_1} \mathcal{R} \mathcal{P} j j' = (N - 2)! \sum_{i} \delta_{i j, \lambda_1} \mathcal{R} \mathcal{P} j j' = (N - 2)! (1 - \delta_{i j, \lambda_1}).$$

Then

$$\Sigma_{jj'}^{(S', S)} = \sum_{\mathcal{R}} D_{[\lambda]}^{[\lambda]} (\mathcal{R}) D_{[\lambda]}^{[\lambda]} (\mathcal{R}) (N - 2)! (1 - \delta_{\lambda_1, \lambda_1})$$

where the last transformation uses Eqs. (5) and (A.1). The last expression in (A.2) is independent of $j$ and $j'$ and equivalent to (34).

The Young orthogonal matrix elements in (A.1) have been calculated by Goddard [33] in the following way. Each permutation $\mathcal{R}$ can be represented as

$$\mathcal{R} = \prod_{k=1}^{n_{NR}} P_{k'u_k}^{(r)} P_{\mathcal{P}'}^{(r')},$$
where $\mathcal{P}'$ are permutations of symbols in the first row of the Young tableau $[0]$ ($\lambda_1$ first symbols), $\mathcal{P}''$ are permutations of symbols in the second row ($\lambda_2$ last symbols), and $\mathcal{P}'_k \mathcal{P}''_k$ transpose symbols between the rows as $i_k' \leq \lambda_1$ and $i_k'' > \lambda_1$. Then for $S, S' \leq \lambda_1$.

Due to the Kronecker symbols in Eq. (A.1), the permutations $\mathcal{P}'$ do not affect $\lambda_1$ and $i_k' \leq \lambda_1 - 1$. Therefore there are $(\lambda_1 - 1)!$ permutations $\mathcal{P}''$, $\lambda_2$! permutations $\mathcal{P}'_k \mathcal{P}''_k$, and number of distinct choices of the sets of $i_k'$ and $i_k''$ are given by the binomial coefficients $\binom{\lambda_1 - 1}{n_{ex}}$ and $\binom{\lambda_2}{n_{ex}}$, respectively. Then for $S = S'$ Eq. (A.1) can be transformed as follows,

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

The sum over $n_{ex}$ can be calculated, leading to (32).

If $S' = S - 1$ we have

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

giving (33).

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