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ANTISYMMETRIZATION PROCEDURE OF IDENTICAL FERMIONS STATES

A. Deveikis[1]

Department of Applied Informatics, Vytautas Magnus University, Kaunas, Lithuania

An efficient procedure for antisymmetrization of an arbitrary system of identical fermions is presented. The approach is based on a simple enumeration scheme for antisymmetric A-particle states and an efficient algorithm for calculation of the coefficients of fractional parentage (CFPs) for a single j-shell with isospin. The developed approach is implemented in a new procedure for the calculation of the electric quadrupole moment matrix elements of light atomic nuclei in the isospin formalism.

Представлена процедура антисимметризации систем идентичных фермионов. Подход основан на простом методе классификации многочастичных состояний и эффективной процедуре расчета одночастичных генеалогических коэффициентов для одной j-орбиты с изоспином. Предлагается использовать только квантовые числа момента, четности, изоспина и одно дополнительное целое квантовое число, предназначенное для классификации антисимметрических состояний. В рамках предложенного подхода реализован новый метод расчета квадрупольных моментов легких ядер в модели ядерных оболочек.

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1. ANTISYMMETRIZATION OF MANY-PARTICLE STATES

The antisymmetric wave function of an arbitrary system of identical fermions may be obtained by calculation of the A-particle antisymmetrization operator matrix Y on the basis of appropriate functions with a lower degree of antisymmetry [1]. The coefficients of fractional parentage are those eigenvectors of the antisymmetrization operator matrix Y that correspond to unit eigenvalues. An efficient algorithm for large-scale calculations of the CFPs for a single j-shell with isospin is presented in [2, 3]. The procedure for constructing of the one-particle multi-shell CFPs from one-particle single-shell CFPs was obtained by Levinsonas [4]. The one-particle multi-shell CFPs enable the antisymmetric A-particle oscillator function to be expressed in the form of linear combinations of vector coupled products of antisymmetric functions of $A-1$ nucleons and one-particle wave functions. The separation of a nucleon from the initial configuration can be accomplished in all possible ways consistent with the required triangular relations, thus giving rise to the general angular momentum recoupling coefficient describing the transformation between different momentum coupling schemes. So, the one-particle multi-shell CFPs definition contains only single-shell CFPs and the corresponding

[1]E-mail: a.deveikis@if.vdu.lt

general angular momentum recoupling coefficient. It should be noted, that any sum over some set of quantum numbers does not appear at all

$$\langle\overline{(EK\Delta J\Pi T)};elj\pi t||EK\Delta J\Pi T\rangle =$$
$$= (-1)^{\nu_r}\left(\frac{n_r}{A}\right)^{1/2}\langle(elj t)_r^{n_r-1}\overline{(\Delta JT)}_r;(elj t)_r||(elj t)_r^{n_r}(\Delta JT)_r\rangle\times$$
$$\times\langle((J_1T_1\ldots\overline{J_rT_r}\ldots J_kT_k)\overline{JT},j_rt_r)JT||(J_1T_1\ldots(\overline{J_rT_r},j_rt_r)J_rT_r\ldots J_kT_k)JT\rangle. \quad (1)$$

In this approach many-particle antisymmetrical states are characterized only by a well-defined set of quantum numbers: the number of oscillator quanta E, configuration K (with specified intermediate coupling), the total angular momentum J, parity π, isospin T, and one additional integer quantum number, Δ, which is necessary for unambiguous enumeration of the states [2]. $(elj)^n$ in Eq. (1) denotes the single shell. The list of occupied shells with the number of nucleons found in each is called a configuration. A single bar over the quantum numbers indicates the parent state, subscript r refers to the rth shell in the configuration, and superscript n_r is the number of particles contained in the rth shell. The specification of single shell is followed by its total momenta and Δ. However, the general angular momentum recoupling coefficient is independent of one-particle quantum numbers and Δ, so their notations are not indicated in its specification. The total momenta of single shells indicated in the general angular momentum recoupling coefficient expression are vector coupled in ascending order if another sequence explicitly displayed by parentheses is not introduced. The integer is $\nu_r = \sum_{i=r+1}^{k} n_i$, where sum runs over all shells standing to the right from the rth shell. $\langle(elj)_r^{n_r-1}\overline{(\Delta JT)}_r;(elj)_r||(elj)_r^{n_r}(\Delta JT)_r\rangle$ denotes the one-particle CFP of the rth shell.

It is well known that the general angular momentum recoupling coefficients with the arbitrary number of the angular momenta can be written explicitly in terms of the Clebsch–Gordan expansion. This can be illustrated with the following example:

$$\langle((j_1,j_2)j_{12},j_3)j|((j_3,j_2)j_{32},j_1)j\rangle =$$
$$= \frac{1}{(2j+1)}\sum_{\substack{m_1m_2m_3\\ m_{12}m_{32}m}}\begin{bmatrix}j_1 & j_2 & j_{12}\\ m_1 & m_2 & m_{12}\end{bmatrix}\begin{bmatrix}j_{12} & j_3 & j\\ m_{12} & m_3 & m\end{bmatrix}\times$$
$$\times\begin{bmatrix}j_3 & j_2 & j_{32}\\ m_3 & m_2 & m_{32}\end{bmatrix}\begin{bmatrix}j_{32} & j_1 & j\\ m_{32} & m_1 & m\end{bmatrix}, \quad (2)$$

where j_1, j_2 and j_3 are the intermediate angular momenta which can, in principle, be coupled to the total angular momentum j in any other way, different from that in the bra- and ket-vectors in the above expression. Expression (2) can be straightforwardly generalized in the case of the arbitrary number and the coupling scheme of angular momenta.

2. ELECTRIC QUADRUPOLE MOMENTS

The electric quadrupole moment operator of an A-nucleon nucleus is defined as

$$\mathbf{Q}_0^{(2)} = \sqrt{\frac{16\pi}{5}}\sum_{i=1}^{A} r_i^2\mathbf{Y}_0^{(2)}(\theta_i,\varphi_i)\,\delta_{m_t(i),-1/2}. \quad (3)$$

Here $\mathbf{Y}_0^{(2)}(\theta_i, \varphi_i)$ is the spherical harmonic of the angular coordinates θ_i and φ_i, and the sum extends over the protons only. In nuclear physics the electric quadrupole moment of an atomic nucleus is defined as the mean value in the substate $M = J$

$$\mathbf{Q} = \langle EK\Delta J\Pi T M_J M_T | \mathbf{Q}_0^{(2)} | EK\Delta J\Pi T M_J M_T \rangle_{M_J=J}. \tag{4}$$

In the impulse approximation, the operator that describes the electromagnetic moment, is a sum of one-particle operators each of which describes the interaction of an independent nucleon with the electromagnetic field

$$\mathbf{Q}_0^{(2)} = \sum_{i=1}^{A} \mathbf{Q}_0^{(2)}(i), \tag{5}$$

here $\mathbf{Q}_0^{(2)}(i)$ refers to the ith particle. Since the wave functions are antisymmetric with respect to all nucleons, all contributions of the summation over i in Eq. (5) to the matrix element of the electric quadrupole moment operator $\mathbf{Q}_0^{(2)}$ are equal. Thus, one may deal only with the last term $\mathbf{Q}_0^{(2)}(A)$

$$\mathbf{Q} = A \, \langle EK\Delta J\Pi T M_J M_T \, | \, \mathbf{Q}_0^{(2)}(A) | \, EK\Delta J\Pi T M_J M_T \rangle_{M_J=J}. \tag{6}$$

The required isolation of particle A from the wave function, more conveniently, may be achieved with the fractional parentage expression of the oscillator shell-model wave function

$$\Phi_{EK\Delta}^{J\Pi T M_J M_T}(x_1 \ldots x_A) = \sum_{\substack{(EK\Delta J\Pi T) \\ elj\pi t}} \langle \overline{(EK\Delta J\Pi T)}; elj\pi t || EK\Delta J\Pi T \rangle \times \\ \times \left\{ \Phi_{\overline{EK\Delta}}^{\overline{J\Pi T}}(x_1 \ldots x_A) \otimes \phi_{el}^{j\pi t}(x_A) \right\}_{J M_J T M_T}. \tag{7}$$

After applying the usual Racah algebra technique, the matrix element of the electric quadrupole moment operator assumes the form convenient for calculation

$$\mathbf{Q} = Ab^2 2 \begin{bmatrix} J & 2 & J \\ J & 0 & J \end{bmatrix} \sqrt{2J+1} \sum_{\substack{(EK\Delta J\Pi T) \\ elj\pi t}} (-1)^{\overline{J}+J-l+\frac{1}{2}} \left(e + \frac{3}{2} \right) (2j+1) \sqrt{2l+1} \times \\ \times \langle \overline{(EK\Delta J\Pi T)}; elj\pi t || EK\Delta J\Pi T \rangle^2 \begin{bmatrix} l & 2 & l \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} j & 2 & j \\ J & \overline{J} & J \end{Bmatrix} \begin{Bmatrix} l & 2 & l \\ j & \frac{1}{2} & j \end{Bmatrix} \times \\ \times \sum_{\overline{M}_T m_t} \begin{bmatrix} \overline{T} & t & T \\ \overline{M}_T & m_t & M_T \end{bmatrix}^2 \delta_{m_t,-1/2}. \tag{8}$$

Here b is the usual oscillator length.

The derived formula (8) was used for calculation of the electric quadrupole moment matrices for all $0p$-shell atomic nuclei in a complete $0\hbar\omega$ basis. The obtained electric quadrupole moment matrix will be labelled by sets of quantum numbers uniquely enumerating the

The quadrupole moments Q of nuclear oscillator A-particle states uniquely characterized by the total angular momentum J and the total isospin T. Here Z is the number of protons

A	Z	JT	**Q**	A	Z	JT	**Q**	A	Z	JT	**Q**
2	1–2	01	0	2	1–2	10	0	3	1–2	$\frac{1}{2}\frac{1}{2}$	0
4	2	00	0	5	2–3	$\frac{1}{2}\frac{1}{2}$	0	5	2	$\frac{3}{2}\frac{1}{2}$	0
5	3	$\frac{3}{2}\frac{1}{2}$	–1	6	2	11	0	6	3	11	–0.25
6	4	11	–0.5	6	3	20	–0.5	6	3	30	–1
7	2–5	$\frac{1}{2}\frac{3}{2}$	0	7	2–5	$\frac{5}{2}\frac{3}{2}$	0	8	2	12	0
8	3	12	0.125	8	4	12	0.25	8	5	12	0.375
8	6	12	0.5	8	3	41	–1	8	4	41	–0.5
8	5	41	0	9	2	$\frac{1}{2}\frac{5}{2}$	0	9	3	$\frac{1}{2}\frac{5}{2}$	0.2
9	4	$\frac{1}{2}\frac{5}{2}$	0.4	9	5	$\frac{1}{2}\frac{5}{2}$	0.6	9	6	$\frac{1}{2}\frac{5}{2}$	0.8
9	7	$\frac{1}{2}\frac{5}{2}$	1	9	2–7	$\frac{3}{2}\frac{5}{2}$	0	10	3–7	02	0
10	2–8	03	0	10	3	32	–1	10	4	32	–0.5
10	5	32	0	10	6	32	0.5	10	7	32	1
10	5	50	0	11	3–8	$\frac{1}{2}\frac{5}{2}$	0	11	3	$\frac{3}{2}\frac{5}{2}$	–1
11	4	$\frac{3}{2}\frac{5}{2}$	–0.8	11	5	$\frac{3}{2}\frac{5}{2}$	–0.6	11	6	$\frac{3}{2}\frac{5}{2}$	–0.4
11	7	$\frac{3}{2}\frac{5}{2}$	–0.2	11	8	$\frac{3}{2}\frac{5}{2}$	0	12	4	1 2	–0.5
12	5	12	–0.375	12	6	12	–0.25	12	7	12	–0.125
12	8	12	0	12	5	41	0	12	6	41	0.5
12	7	41	1	13	5–8	$\frac{1}{2}\frac{3}{2}$	0	13	5–8	$\frac{5}{2}\frac{3}{2}$	0
14	7	30	1	14	6	11	0.5	14	7	11	0.25
14	8	11	0	14	7	20	0.5	15	7–8	$\frac{1}{2}\frac{1}{2}$	0
15	7	$\frac{3}{2}\frac{1}{2}$	1	15	8	$\frac{3}{2}\frac{1}{2}$	0	16	8	00	0

corresponding states. Among these are: shells constituting the configuration, intermediate momenta, and Δs. Obviously, wave functions from subspaces characterized by the mentioned quantum numbers should mix, when any real interaction is involved. So, the reasonable result can be obtained only after diagonalization of the Hamiltonian matrix in the corresponding subspace. The only exception is when total J and T uniquely characterize the A-particle state, i.e., when the dimension of the subspace is one. The electric quadrupole moments of such states are presented in the Table. For better comprehension of the obtained results the oscillator length b was taken as equal to one, and the free-space values of the proton and neutron charges were used. The calculation data coincide with extreme-single-particle model predictions, in the cases where this model can be applied.

CONCLUSION

In this paper we present a new formula and procedure for the calculation of the electric quadrupole moment matrix elements of light atomic nuclei in the isospin formalism. The proposed procedure consistently outlines the principle of antisymmetrization. A distinct feature of this procedure is in the complete rejection of group-theoretical classification of antisymmetric many-particle states. This is a remarkable circumstance, because a benefit could be gained due to simplicity and comprehensibility of such a kind of calculations. The method is based on the observation that multi-shell coefficients of fractional parentage can be expressed in terms of single-shell CFPs [4]. The latter are calculated using the algorithm [2] for a spectral decomposition of an antisymmetrization operator matrix Y. The calculation procedures for the evaluation of the electric quadrupole moments have been implemented in the computer code and the electric quadrupole moment matrices for all $0p$-shell atomic nuclei in a complete $0\hbar\omega$ basis were calculated. The presented approach could be tailored for an arbitrary system of identical fermions.

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