

Table of Sanibel (Spin Projection) Coefficients*

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Projection coefficients for total spin angular momentum of systems of 1 to 20 particles with spin $\frac{1}{2}$ have been calculated on a digital computer.

Die Projektionskoeffizienten für Eigenzustände des Betrages des Spindrehimpulses sind für Systeme von 1 bis 20 Spin- $\frac{1}{2}$ -Teilchen berechnet worden.

Les coefficients de projection du moment angulaire de spin total de systèmes de 1 à 20 particules de spin $\frac{1}{2}$ ont été calculés sur un ordinateur.

Introduction

For the construction of angular momentum eigenfunctions the projection operator formalism developed by LÖWDIN [2] is a useful alternative to conventional group theoretical methods. In connection with methods of "different orbitals for different spins", where the trial wave function in general does not represent a pure spin state, spin projection operators are of great importance. The name Sanibel coefficients for their expansion coefficients was coined by PAUNZ in connection with the 1962 quantum theory symposium on Sanibel Island, Florida, where the first results for $S \neq 0$ were discussed [3].

Since explicit formulas are now available for arbitrary values of S and $M = S_z$, a table of Sanibel coefficients was thought to be useful for further work in this field. For that purpose we have calculated on a digital computer the Sanibel coefficients for 1 to 20 particles with spin $\frac{1}{2}$. Due to space limitations we present here only the first part of the table, for 1 to 10 particles. The full table for 1 to 20 particles is however available in mimeographed form from the Uppsala Quantum Chemistry Group as Technical Note No. 153, June 15, 1965, (62 pages).

Theory

Let us consider an N -particle Slater-determinant

$$\Phi = \mathcal{A} a_1(1) \alpha(1) \dots a_\mu(\mu) \alpha(\mu) b_1(\mu+1) \beta(\mu+1) \dots b_\nu(N) \beta(N). \quad (1)$$

One obtains immediately the z -component of spin as $M = (\mu - \nu)/2$ and, without lack of generality, we restrict ourselves to determinants with $M \geq 0$. In general Φ

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Table

$N=2n$	S	M	j	C	$N=2n$	S	M	j	C	
1	0.5	0.5	0	1	6	1	1	0	3/5	
2	0	0	0	1/2	2	2	0	1	-3/20	
			1	-1/2				2	1/10	
			0	1/2				0	1/4	
			1	1/2				1	1/12	
3	0.5	0.5	0	2/3	2	1	0	2	-1/12	
			1	-1/3				3	-1/4	
			0	1/3				0	1/3	
			1	1/3				1	1/12	
4	0	0	0	1/3	3	1	0	2	-1/6	
			1	-1/6				0	5/6	
			2	1/3				1	-1/6	
			0	1/2				0	1/20	
5	0.5	0.5	0	1/2	3	2	0	1	1/20	
			1	-1/6				2	1/20	
			2	1/6				3	1/20	
			0	2/5				0	1/15	
			1	1/15				1	1/15	
			2	-4/15				2	1/6	
	1.5	0.5	0.5	0	2/5	3	2	0	1	1/6
				1	1/15				0	3/4
				2	-4/15				1	-1/4
				0	4/5				0	1/6
				1	-1/5				1	1/6
				2	1/10				2	1/6
2.5	0.5	0.5	0	1/10	3	3	2	0	1/6	
			1	1/10				0	1/6	
			2	1/10				1	1/6	
			0	1/5				0	1/4	
			1	-1/5				1	1/4	
			2	1/10				2	1/4	
3.5	1.5	1.5	0	1/5	3	3	3	0	1/6	
			1	1/5				1	1/6	
			2	1/5				2	1/6	
			0	1				0	1/6	
			1	1				1	1/6	
			2	1				2	1/6	
6	0	0	0	1/4	7	0.5	0.5	0	2/5	
			1	-1/12				1	-1/10	
			2	1/12				2	1/15	
			3	-1/4				3	-1/10	
			0	9/20				0	2/5	
			1	-1/20				1	0	
	1	0	0	0	9/20	1.5	0.5	0.5	2	-1/15
				1	-1/20				3	1/5
				2	-1/20				0	2/3
				3	9/20				1	-2/15
				0	1				2	1/15
				1	1				0	6/35
2.5	1.5	1.5	0	1/5	2.5	0.5	0.5	1	1/14	
			1	1/5				1	-1/35	
			2	1/5				2	-1/35	
			0	1/10				3	-9/70	
			1	1/10				0	2/7	
			2	1/10				1	3/35	
3.5	2.5	2.5	0	1/5	3.5	1.5	1.5	2	-4/35	
			1	1/5				0	6/7	
			2	1/5				1	-1/7	
			0	1				0	1/35	
			1	1				1	1/35	
			2	1				2	1/35	
4.5	3.5	3.5	0	1	3.5	2.5	2.5	0	1/7	
			1	1				1	1/7	
			2	1				2	1/7	
			0	1				0	1	
			1	1				1	1	
			2	1				2	1	

Table (continuation)

$N=2n$	S	M	j	C	$N=2n$	S	M	j	C
8	0	0	0	1/5	8	4	4	0	1
			1	-1/20				1	1/3
			2	1/30				1	-1/15
			3	-1/20				2	1/30
			4	1/5				3	-1/30
	1	0	0	2/5		4	1/15		
			1	-1/20		0	8/21		
			2	0		1.5	0.5	1	-2/105
			3	1/20		1	-2/105		
			4	-2/5		2	-2/105		
	1	1	0	1/2		3	1/21		
			1	-1/10		4	-16/105		
			2	1/20		1.5	1.5	0	4/7
			3	-1/20		1	-2/21		
			4	1/28		2	4/105		
2	0	0	2/7	3	-1/35				
		1	1/28	2.5	0.5	0	3/14		
		2	-1/21	1	3/70				
		3	1/28	2	-1/35				
		4	2/7	3	0				
2	1	0	5/14	4	9/70				
		1	1/42	2.5	1.5	0	9/28		
		2	-5/84	1	1/28				
		3	3/28	2	-1/20				
		4	5/7	3	9/140				
2	2	0	5/7	2.5	2.5	0	3/4		
		1	-5/42	1	-3/28				
		2	1/21	2	1/28				
		3	3/28	3	-1/20				
		4	5/7	4	9/140				
3	0	0	1/10	3.5	0.5	0	4/63		
		1	1/20	1	11/315				
		2	0	2	2/315				
		3	-1/20	3	-1/45				
		4	-1/10	4	-16/315				
3	1	0	1/8	3.5	1.5	0	2/21		
		1	7/120	1	1/21				
		2	-1/120	2	0				
		3	-3/40	3	-1/21				
		4	1/4	4	2/9				
3	2	0	1/4	3.5	2.5	0	5/63		
		1	1/12	1	-4/63				
		2	-1/12	2	8/9				
		3	7/8	1	-1/9				
		4	-1/8	4.5	0.5	0	1/126		
4	0	0	1/70	1	1/126				
		1	1/70	2	1/126				
		2	1/70	3	1/126				
		3	1/70	4	1/126				
		4	1/70	4.5	1.5	0	1/84		
4	1	0	1/56	1	1/84				
		1	1/56	2	1/84				
		2	1/56	3	1/84				
		3	1/56	4.5	2.5	0	1/36		
		4	1/56	1	1/36				
4	2	0	1/28	2	1/36				
		1	1/28	3	1/36				
		2	1/28	4	1/36				
		3	1/28	1	1/36				
		4	1/28	2	1/36				
4	3	0	1/8	1	1/36				
		1	1/8	2	1/36				

Table (continuation)

$N=2n$	S	M	j	C	$N=2n$	S	M	j	C	
9	4.5	3.5	0	1/9	10	3	2	0	7/24	
			1	1/9				1	1/24	
	0	1	2	-1/24						
		3	1/24							
		0	7/9							
	4.5	4.5	0	1			3	3	0	-7/72
10	0	0	0	1/6			4	0	0	1/28
			1	-1/30		1			3/140	
			2	1/60		2			1/140	
			3	-1/60		3			-1/140	
			4	1/30	4	-3/140				
			5	-1/6	5	-1/140				
					0	5/14				
					1	-3/70				
					2	1/140				
					3	1/140				
		1	0	0	5/14		4	1	0	3/70
				1	-3/70	1			1/40	
				2	1/140	2			1/140	
				3	-3/70	3			-3/280	
				4	5/14	4			-1/35	
				5	3/7	5			3/40	
				0	-1/14				11/280	
				1	1/35				1/280	
				2	-3/140				-9/280	
				3	1/35				1/5	
		1	1	0	25/84		4	3	0	3/40
				1	1/84	1			2	
				2	-1/42	2			-1/20	
				3	1/42	3			9/10	
				4	-1/84	4			-1/10	
				5	-25/84	5			0	
				0	5/14				1/252	
				1	0				1/252	
				2	-1/42				1/252	
				3	1/28				1/252	
		4	-1/14		1/252					
	2	2	0	5/8		5	1	0	1/210	
			1	-5/56	1			1/210		
			2	5/168	2			1/210		
			3	-1/56	3			1/210		
			0	5/36				1/210		
			1	7/180				1/210		
			2	-1/90				1/120		
			3	-1/90				1/120		
			4	7/180				1/120		
			5	5/36				1/45		
	3	0	0	5/36		5	2	0	1/120	
			1	7/180				1/120		
			2	-1/90				1/120		
			3	-1/90				1/120		
			4	7/180				1/120		
			5	5/36				1/45		
			0	1/6				1/45		
			1	1/24				1/45		
			2	-1/60				1/10		
			3	-1/120				1/10		
	3	1	0	1/6		5	5	0	1	
			1	1/24						
			2	-1/60						
			3	-1/120						
		4	1/15					0	1	

is not an eigenfunction of total spin but represents a mixture of spin states ranging from $S = M$ up to $S = N/2$ with integer intervals. The projection operator O_S selects from Φ the component with the desired total spin S .

A general form of a projection operator associated with the eigenvalue λ_k of the operator Λ is

$$O_k = \prod_{l \neq k} \frac{\Lambda - \lambda_l}{\lambda_k - \lambda_l}. \quad (2)$$

Here each factor $(\Lambda - \lambda_l)$ annihilates the component associated with the eigenvalue λ_l . From (2) it is easy to obtain relations characteristic of projection operators, e.g.

$$O^2 = O \quad \text{and} \quad \sum_{\text{all } k} O_k = 1 \quad (3)$$

the latter being useful in this context for checking purposes. Since the antisymmetrizer $\mathcal{A} = (N!)^{-1/2} \sum_P (-1)^P P$ commutes with spin operators S^2 and O_S and these leave the space part of the wavefunction unchanged we simplify our expressions by considering a trial function composed of a product of α and β spin functions

$$\chi = [\alpha^\mu] [\beta^\nu]. \quad (4)$$

As shown by LÖWDIN [2] the projected spin function can be written as

$$O_S \chi = \sum_{j=0}^{\nu} C_j(S, M, n) [\alpha^{\mu-j} \beta^j] [\alpha^j \beta^{\nu-j}]. \quad (5)$$

The coefficients $C_j(S, M, n)$ are the Sanibel coefficients, n denoting half the number of particles ($n = N/2$), and $[\alpha^p \beta^q]$ is the sum of all products of p α -functions and q β -functions. In order to construct the full trial function the first bracket should be multiplied by the μ a -functions, the second one by the product of the ν b -functions in (1), and the whole expression has finally to be antisymmetrized.

Analytical expressions for Sanibel coefficients have been obtained by, among others, LÖWDIN and PAUNZ [3], SASAKI and OHNO [5], PERCUS and ROTENBERG [4] and SMITH [6]. Here we cite only SMITH's generalization of the PERCUS and ROTENBERG expression

$$C_j(S, M, n) = \frac{2S+1}{1+n+S} \sum_{k=0}^{S-M} (-1)^{j+S-M-k} \binom{S-M}{k} \binom{S+M}{S-M-k} \binom{n+S}{\mu-j+k}^{-1} \quad (6)$$

and the recursion relation derived by HARRIMAN [1]

$$C_j(S, M, n) - C_{j+1}(S, M, n) = C_j(S, M, n-1) \quad (7)$$

which have been used in the present numerical calculation.

Numerical procedure

Programs were written in Fortran IV and run at the IBM 7090 computer at the Swedish Research Institute for National Defense, Stockholm. In order to obtain exact results fractional numbers were represented by their integer numerators and denominators and the arithmetic processing of these was done by fixed-point subroutines. Euclid's algorithm was used to find the largest common factors for cancelling. For a given S and M the Sanibel coefficients were first evaluated for $n = S$ using formula (6). For $n = S + 1, S + 2 \dots$ the same relation was used in the case of $j = 0$ followed by the recursion relation (7) for higher j -values. Relation (3b) was checked in double precision floating point. A listing of the complete source program is available at this institute.

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