Moshinsky brackets for light nuclei

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A new formula for calculation of the Moshinsky brackets is derived. As its consequence, simple formulas for the angle-averaged Pauli projector matrix elements and for the transformed two-particle oscillator wave functions are given.

[NUCLEAR STRUCTURE New formulas for Moshinsky brackets, Pauli projector and Moshinsky transformed states.]

I. INTRODUCTION

The well-known two-particle oscillator wave functions

$$\langle \vec{r}_1 \vec{r}_2 | n_1 l_1 n_2 l_2 \lambda \mu \rangle = R_{n_1 l_1}(r_1) R_{n_2 l_2}(r_2) \sum_{m_1 m_2} C^{\lambda\mu}_{l_1 m_1 l_2 m_2} Y_{l_1 m_1}(\vartheta_1, \varphi_1) Y_{l_2 m_2}(\vartheta_2, \varphi_2) \tag{1}$$

(see Ref. 1) constitute the basis in the two-nucleon space. In practice[1,2] the eigenket $|n_1 l_1 n_2 l_2 \lambda \mu\rangle$ is frequently expressed in the relative and center-of-mass coordinates (RCM)

$$\vec{r} = 2^{-1/2}(\vec{r}_1 - \vec{r}_2), \quad \vec{R} = 2^{-1/2}(\vec{r}_1 + \vec{r}_2).$$

The well-known Moshinsky transformation[2] leads to the expansion

$$\langle \vec{r}\vec{R} | n_1 l_1 n_2 l_2 \lambda \mu \rangle = \sum_l \psi_i(r, R) \sum_{mM} C^{\lambda\mu}_{lmLM} Y_{lm}(\vartheta, \varphi) Y_{LM}(\Theta, \Phi), \quad i \equiv \{n_1 l_1 n_2 l_2 l L \lambda\}, \tag{2}$$

where the partial waves

$$\psi_i(r, R) = \sum_{nN} (nl, NL; \lambda | n_1 l_1, n_2 l_2; \lambda)_1 \times R_{nl}(r) R_{NL}(R) \tag{3}$$

may easily be calculated, once the Moshinsky brackets (MB) $(nl, NL; \lambda | n_1 l_1, n_2 l_2; \lambda)_1$ are known.[2,3]

In the present paper, we shall suppose the restriction

$$2n_1 + l_1 \le F \tag{4}$$

and investigate the possibilities of optimal calculation of MB. The main motivation issues from the Brueckner theory[1] where the condition Eq. (4) defines the occupied (hole) state and where hole-hole ($|hh'\rangle$) and hole-particle ($|hp\rangle$) oscillator functions of the type Eq. (2) are needed to define the Pauli projector[1]

$$Q = 1 - P = Q^2, \quad P|hh'\rangle = |hh'\rangle, \quad P|hp\rangle = |hp\rangle, \quad P|pp'\rangle = 0. \tag{5}$$

The oscillator approximation (1) for $|hh'\rangle$ and $|hp\rangle$ functions is well founded in light nuclei only: The value F should be 0 in ^{4}He, 1 (^{16}O), 2 (^{40}Ca) etc., so that the formula for MB, optimal for low F, is very desirable. Such a formula is derived in Sec. II. It is employed to obtain the formula for the angle-averaged Pauli projector (Sec. III) and the expression for the functions of the type (3) (uncorrelated oscillator wave functions, Sec. IV).

II. NEW FORMULA FOR MOSHINSKY BRACKETS

Our starting point will be the formula derived by Trlifaj[4]

$$(nl,NL;\lambda|n_1l_1,n_2l_2;\lambda)_D=(-1)^{n_1+n_2+n+\lambda}2^{-1}\pi^{1/2}(1+D^{-1})^{-l/4}(1+D)^{-l/4}$$
$$\times(2l+1)\left\{\frac{n!n_1!n_2!\Gamma(n_1+l_1+3/2)\Gamma(n_2+l_2+3/2)}{N!\Gamma(n+l+3/2)\Gamma(N+L+3/2)}\right\}^{1/2}\delta(2n+l+2N+L,2n_1+l_1+2n_2+l_2)$$
$$\times\sum_{\substack{p_1m_1\lambda_1\\p_2m_2\lambda_2}}(-1)^{\lambda_1+m_1+m_2+(p_1+p_2+L)/2}D^{(\lambda_2-\lambda_1)/4}(1+D^{-1})^{-m_1-p_1/2}\binom{2l}{2\lambda_1}^{1/2}\begin{Bmatrix}p_1 & p_2 & L\\ \lambda_1 & \lambda_2 & l\\ l_1 & l_2 & \lambda\end{Bmatrix}$$
$$\times\frac{(2p_1+1)(2p_2+1)C^{l_1}_{p_1\lambda_1}C^{l_2}_{p_2\lambda_2}C^{L}_{p_1p_2}\,\delta(\lambda_1+\lambda_2,l)}{(1+D)^{m_2+p_2/2}m_1!\Gamma(p_1+m_1+3/2)m_2!\Gamma(p_2+m_2+3/2)}$$
$$\times\frac{[\frac{1}{2}(p_1+p_2-L)+m_1+m_2]!\Gamma[\frac{1}{2}(p_1+p_2+L)+m_1+m_2+3/2]}{[n_1-\frac{1}{2}(\lambda_1+p_1-l_1)-m_1]![n_2-\frac{1}{2}(\lambda_2+p_2-l_2)-m_2]![\frac{1}{2}(p_1+p_2-L)+m_1+m_2-N]!},\quad(6)$$

which expresses MB for any mass ratio $D=M_1/M_2$ in the form of the sum over five independent variables. The summation is restricted by the existence of factorials, Clebsch-Gordan coefficients[5]

$$C^{l_3}_{l_1l_2}\equiv C^{l_30}_{l_10l_20}$$

and a 9-j symbol[5]

$$\begin{Bmatrix}\cdot\cdot\cdot\\ \cdot\cdot\cdot\\ \cdot\cdot\cdot\end{Bmatrix}.$$

Let us suppose that one of the energy quantum numbers $E_i=2n_i+l_i$ is small. Using the symmetry[2] of MB, we put $E_1=E_{\text{minimal}}$ and introduce new (non-negative) summation variables μ, ρ, and ν instead of p_1, p_2, and λ_1, respectively, following the prescription

$$p_1=\mu+\nu,\quad p_2=2\rho+L-p_1,\quad \lambda_1=2\nu+l_1-p_1.$$

The triangular inequalities for the triads $(p_1\lambda_1l_1)$ and (p_1p_2L) and the existence of the factorial containing the variable ν imply

$$0\le\mu\le l_1,$$
$$0\le\nu\le n_1,$$
$$0\le\rho\le\mu+\nu,$$
$$0\le m_1\le n_1-\nu.$$

Thus the number $M(n_1,l_1)$ of terms in the sum over p_1, p_2, λ_1, λ_2, and m_1 is limited by the condition

$$M(n_1,l_1)\le\tfrac{1}{12}(l_1+1)(n_1+1)(n_1+2)(2n_1+3l_1+6)$$

and we have $M(0,0)\le1$, $M(0,1)\le3$, $M(1,0)\le4$, $M(0,2)\le6,\ldots$. No similar condition, limiting the number of terms, can be found for the sum over the remaining index m_2. It would be very desirable to perform this summation in an explicit way.

With this intention, we introduce the auxiliary function $W^{\alpha\beta}_{LD}(N,m)$ by the prescription

$$W^{\alpha\beta}_{LD}(N,m)=\sum_{k=0}^{m}\frac{(-1)^kD^{\alpha+\beta-m}}{(1+D)^{k-m}}\binom{m}{k}\times\frac{\Gamma(N+k+1)\Gamma(N+k+L+3/2)}{\Gamma(N-\alpha+k+1)\Gamma(N-\beta+k+L+3/2)}\quad(7)$$

and suppose that $N+1-\alpha\ne0,-1,\ldots$. It is clear that for $\alpha=\beta=0$, Eq. (7) is the familiar binomial expansion, i.e.,

$$W^{00}_{LD}(N,m)=1,\quad m\ge0,$$
$$W^{00}_{LD}(N,m)=0,\quad m<0.\quad(8)$$

For $\alpha\ne0$ or $\beta\ne0$ we have the recurrence relations

$$W^{\alpha+1\beta}_{LD}(N,m)=D(N-\alpha)W^{\alpha\beta}_{LD}(N,m)-mW^{\alpha\beta}_{LD}(N+1,m-1),$$
$$W^{\alpha\beta+1}_{LD}(N,m)=D(N-\beta+L+1/2)W^{\alpha\beta}_{LD}(N,m)-mW^{\alpha\beta}_{LD}(N+1,m-1),\quad m\ge0\quad(9)$$

that enable us to write down the explicit forms of the polynomials W, e.g.,

$$W^{10}_{LD}(N,m)=DN-m,$$
$$W^{01}_{LD}(N,m)=W^{10}_{LD}(N+L+\tfrac{1}{2},m),$$
$$W^{20}_{LD}(N,m)=D^2N(N-1)-2DNm+m(m-1),$$
$$W^{02}_{LD}(N,m)=W^{20}_{LD}(N+L+\tfrac{1}{2},m),\quad(10)$$
$$W^{11}_{LD}(N,m)=D^2N(N+L+\tfrac{1}{2})-Dm(2N+L+\tfrac{3}{2})+m(m-1),$$

etc. (see Appendix). We use this function W instead of the sum over m_2 in Eq. (6) and after some elementary algebraic manipulations we obtain the general formula for MB in the form of the sum

$$(nl,NL;\lambda|n_1l_1,n_2l_2;\lambda)_D=\phi_D(N,n)\sum_{\nu=0}^{n_1}\sum_{\mu=0}^{l_1}\sum_{\rho=0}^{\mu+\nu}\begin{Bmatrix}p_1 & p_2 & L\\ \lambda_1 & \lambda_2 & l\\ l_1 & l_2 & \lambda\end{Bmatrix}(-1)^\lambda a(\nu,\mu,\rho)B_D(\mu,\nu,\rho,N,n), \tag{11}$$

$$B_D(\mu,\nu,\rho,N,n)=\sum_{m_1=0}^{n_1-\nu}\frac{(1+D)^{n_1-\nu-m_1}\Gamma(3/2)b_D(m_1,N,n)}{m_1!(n_1-\nu-m_1)!\Gamma(p_1+m_1+3/2)}.$$

Here, the quantity ϕ denotes the normalization factor

$$\phi_D(N,n)=(-1)^{(L+l_2-l-l_1)/2}\delta(2n+l+2N+L,2n_1+l_1+2n_2+l_2)$$
$$\times\frac{D^{(2n+l-2n_1-l_1)/2}}{(1+D)^{(2n_1+l_1+2n_2+l_2)/2}}\left\{\frac{n_1!n_2!\Gamma(n_1+l_1+3/2)\Gamma(n_2+l_2+3/2)}{n!N!\Gamma(n+l+3/2)\Gamma(N+L+3/2)}\right\}^{1/2},$$

the Clebsch-Gordan coefficients are contained in

$$a(\nu,\mu,\rho)=(-1)^{p_1}(2l+1)(2p_1+1)(2p_2+1)\binom{2l}{2\lambda_1}^{1/2}C^{l_1}_{p_1\lambda_1}C^{l_2}_{p_2\lambda_2}C^{L}_{p_1p_2},$$

and the factor $b_D(m_1)$ is given in terms of the auxiliary function W

$$b_D(m_1,N,n)=(-1)^{q_1}\frac{n!}{(n-n_1+\nu+m_1+q_1)!}W_{LD}^{\rho+m_1+q_1,\,p_1-\rho+m_1}(N,n-n_1+\nu+m_1+q_1),\qquad q_1=\min(N-\rho-m_1,0).$$

The same factor $b_D(m_1,N,n)$ will be obtained with $q_1=0$: This property follows directly from Eq. (9), when we define the sum (7) for integer $\alpha>N$ by restriction $k\ge\alpha-N$. Thus, with respect to N,n, the function $b_D(m_1,N,n)$ is a polynomial. Since the degree of this polynomial is equal to

$$\alpha+\beta+n_1-\nu-m_1=n_1+m_1+\mu\le 2n_1+l_1=E_1,$$

the short table of W [e.g., Eq. (10) for $E_1\le 2$, i.e., for nuclei up to ^{40}Ca] is entirely sufficient for its evaluation when E_1 is bounded. In computer code,[3] the further summations are hidden also in the calculation of 9-j and $a(\nu,\mu,\rho)$ coefficients. We should employ all possibilities of their reduction (c.f. $l=0$ in Ref. 4). Since a significant simplification always takes place for the lowest E_1, we now add the reduced forms of Eq. (11) with $E_1=0$ and 1.

In the case of $n_1=l_1=0$, the sum (11) reduces to one term. We get

$$(nl,NL;\lambda|00,n_2l_2;\lambda)_D=\phi_D(N,n)\left\{\frac{(2l+1)(2L+1)}{(2l_2+1)}\right\}^{1/2}(-1)^\lambda\delta_{\lambda,l_2}C^{l_2}_{Ll}. \tag{12}$$

It is interesting to note that $(nl,NL;\lambda|n_2l_2,00;\lambda)_D\ge 0$.

The next energy shell has the quantum numbers $n_1=0$, $l_1=1$ and the number of terms in Eq. (11) is equal to three. We get

$$(nl,NL;\lambda|01,n_2l_2;\lambda)_D=\phi_D(N,n)[\tfrac{1}{3}(2l+1)]^{1/2}\left[a\begin{Bmatrix}L & l & \lambda\\ 1 & l_2 & l-1\end{Bmatrix}+b\begin{Bmatrix}l & L & \lambda\\ 1 & l_2 & L-1\end{Bmatrix}+c\begin{Bmatrix}l & L & \lambda\\ 1 & l_2 & L+1\end{Bmatrix}\right], \tag{13}$$

where

$$a=(-1)^\lambda C^{l_2}_{Ll-1}\{(2L+1)(2l+1)l(2l-1)\}^{1/2},\qquad b=(-1)^{l_2}C^{l_2}_{L-1l}\{4L(2L-1)\}^{1/2}[D(N+L+\tfrac{1}{2})-n],$$

$$c=(-1)^{l_2}C^{l_2}_{L+1l}\{4(L+1)(2L+3)\}^{1/2}[n-DN],$$

and $\{\because\}$ denotes the 6-j symbol.[5] Similar formulas may be written also for $E_1=2$; the use of the algebraic tables[5] makes possible the evaluation of angular coefficients (for $E_1\le 2$) in a square root form.

III. PAULI PROJECTOR

In order to avoid the coupling of equations for the reaction matrix in the Brueckner theory,[1] the Pauli projector (5) is often approximated by its angle-averaged form,[1] defined as

$$\bar{Q}=1-\sum_{\substack{nn'l\\NN'L}}|nl,NL\rangle\Big[\sum_{n_1l_1n_2l_2}w_{n_1l_1n_2l_2}P^{nn'l}_{NN'L}(n_1l_1n_2l_2)\Big]\langle n'l,N'L|, \tag{14}$$

where

$$P^{nn'l}_{NN'L}(n_1l_1,n_2l_2)=\sum_{\lambda=|L-l|}^{L+l}\frac{(2\lambda+1)}{(2L+1)(2l+1)}(nl,NL;\lambda|n_1l_1,n_2l_2;\lambda)_1(n'l,N'L;\lambda|n_1l_1,n_2l_2;\lambda)_1 \tag{15}$$

and $w_{n_1l_1n_2l_2}$ corresponds to occupation probability. In this section we suggest, in the evaluation of Eq. (15), the use of the explicit formulas based on Eq. (11).

The first argument in favor of such an approach is valid for all nuclei: The summation over λ may be performed in an analytic way. From Eq. (11) we get

$$P^{nn'l}_{NN'L}(n_1l_1n_2l_2)=\phi_1(N,n)\phi_1(N',n')\sum_{\nu\mu\rho}a(\nu,\mu,\rho)B_1(\nu,\mu,\rho,N,n)\sum_{\nu'\mu'\rho'}a(\nu',\mu',\rho')B_1(\nu',\mu',\rho',N',n')$$
$$\times(2l+1)^{-1}(2L+1)^{-1}\begin{bmatrix}p_1 & p_1' & \lambda_2 & \lambda_2'\\ p_2 & \lambda_1 & p_2' & \lambda_1'\\ L & l_2 & l_1 & l\end{bmatrix}, \tag{16}$$

where $\begin{bmatrix}\cdot\cdot\cdot\cdot\\ \cdot\cdot\cdot\cdot\\ \cdot\cdot\cdot\cdot\end{bmatrix}$ denotes the 12-j symbol of the second kind.[5] The 12-j symbol introduces nontrivial restrictions[6] (e.g., triangular and quadrangular inequalities) into sum (16).

As the second argument, let us demonstrate the efficiency of this approach in more detail for nuclei up to ^{16}O. For $n_1=0, l_1=1$ we get the special form of Eq. (16) from Eqs. (13) and (15)

$$P^{nn'l}_{NN'L}(01n_2l_2)=\frac{\phi_1(N,n)\phi_1(N',n')}{3(2L+1)}\sum_\lambda(2\lambda+1)\left[a^2\begin{Bmatrix}l & L & \lambda\\ l_2 & 1 & l-1\end{Bmatrix}^2+a(b+b')\begin{Bmatrix}L & l & \lambda\\ 1 & l_2 & l-1\end{Bmatrix}\begin{Bmatrix}L & l & \lambda\\ l_2 & 1 & L-1\end{Bmatrix}+\cdots\right].$$

The sum over λ may be evaluated in terms of 6-j symbols again. Using the formulas of Ref. 5 we finally get

$$P^{nn'l}_{NN'L}(01,n_2l_2)=\frac{\phi_1(N,n)\phi_1(N',n')}{6(2L+1)}\Big[\frac{2a^2}{2l-1}+\frac{2bb'}{2L-1}+\frac{2cc'}{2L+3}-\{[(l_2+L)^2-l^2][(l_2+1)^2-(l-L)^2]\}^{1/2}$$
$$\times C^{l_2}_{Ll-1}C^{l_2}_{L-1l}[D(N+N'+2L+1)-n-n']$$
$$-\{[(l+L+1)^2-l_2^2][(l+L+1)^2-(l_2+1)^2]\}^{1/2}C^{l_2}_{Ll-1}C^{l_2}_{L+1l}[D(N+N')-n-n']\Big], \tag{17}$$

where the symbols a,b,c are given in Eq. (13).

An even more elementary formula is obtained in the case of $n_1=l_1=0$, namely

$$P^{nn'l}_{NN'L}(00,n_2l_2)=\phi_1(N,n)\phi_1(N',n')(C^{l_2}_{Ll})^2, \tag{18}$$

because the Kronecker δ entirely eliminates the angle averaging.

The results may then be inserted into the definition (14) of P, where the factor $w_{n_1l_1n_2l_2}$ should be calculated in a self-consistent way. For a magic nucleus, occupation probability may be assumed to be fixed.[1] The choice

$$w_{n_1l_1n_2l_2}=\delta_{n_1,0}\delta_{l_1,0}+\delta_{n_2,0}\delta_{l_2,0}-\delta_{n_1,0}\delta_{l_1,0}\delta_{n_2,0}\delta_{l_2,0} \tag{19}$$

corresponds to ^{4}He. Let us use this nucleus as an example: For convenience, we put $N'=N$ and $l\geq L, l-L=q$ and get

$$\langle nl,NL|1-\bar{Q}|n'l,NL\rangle$$
$$=\delta_{nn'}\frac{(2-\delta_{n,0}\delta_{N,0}\delta_{l,0}\delta_{L,0})\Gamma(3/2)2^{-q}}{4^{n+N+L}\Gamma(n+l+3/2)\Gamma(N+L+3/2)}$$
$$\times\sum_{m=0}^{L}(n+N+L-m)!\,\Gamma(n+N+l+m+3/2)(C^{2m+q}_{Ll})^2. \tag{20}$$

The other cases $(N'\neq N, l<L)$ are quite analogous.

Even from the physical point of view, the approximation of Q by its diagonal part is considered to be reasonable since it leads to further decoupling of the Bethe-Goldstone equation (see Ref. 1). In the first order calculation of ^{4}He, it is then necessary to consider just $N=L=0$. Since formula (20) in this case reduces to the elementary expression

$$\langle nl00|1-\bar{Q}|n'l'00\rangle=\delta_{nn'}\delta_{ll'}\frac{2-\delta_{n,0}\delta_{l,0}}{2^{2n+l}}, \tag{21}$$

there is no trouble with MB at all. The situation in the next shells may be treated in a similar way.

IV. UNCORRELATED WAVE FUNCTIONS

A. Moshinsky transformation

In Ref. 7, the method of calculation of the Brueckner correlated function $|\psi\rangle$ with exact treatment of Pauli projector Q [Eq. (5)] was suggested and described. The method is based on the knowledge of the uncorrelated oscillator wave functions of the hole-hole $|hh'\rangle$ and hole-particle $|hp\rangle$ type in RCM variables. Since these functions may be of more general interest, we shall now show their compact form that may be derived from formula (11). Referring to the angular momentum coupling, as discussed in Ref. 7, we confine ourselves to radial parts, functions (3).

Our present aim is to show how the summation over oscillator quantum numbers n and N may be performed. According to Eq. (11), the explicit n, N dependence of MB is of the type $(nl,NL;\lambda|n_1l_1,n_2l_2;\lambda)_D$ = polynomial (n,N) $\times\phi_D(N,n)=p_i(n,N)\phi_D(N,n)$ where the composite index $i=\{n_1l_1n_2l_2lL\lambda\}$ determines the form of the polynomial

$$p_i(n,N)=(nl,NL,\lambda|n_1l_1,n_2l_2;\lambda)_D/\phi_D(N,n)$$
$$=\sum_{\nu\mu\rho}(-1)^\lambda a(\nu,\mu,\rho)\begin{Bmatrix}p_1 & p_2 & L\\ \lambda_1 & \lambda_2 & l\\ l_1 & l_2 & \lambda\end{Bmatrix}$$
$$\times B_D(\nu,\mu,\rho,N,n) \qquad (22)$$

of degree $E_1=2n_1+l_1$. Inserting this into Eq. (3), we get

$$\psi_i(r,R)=\text{const}\times r^lR^L\exp[-\tfrac{1}{2}(r^2+R^2)]\varphi_{00}^{ilL}(r^2,R^2), \qquad (23)$$

where the functions

$$\varphi_{ab}^{ilL}(x,y)=\sum_{n+N=M}p_i(n-a,N-b)$$
$$\times\frac{L_n^{l+1/2}(x)L_N^{L+1/2}(y)z^N}{\Gamma(n+l+3/2)\Gamma(N+L+3/2)}, \qquad (24)$$
$$z=D,\quad M=n_1+n_2+\tfrac{1}{2}(l_1+l_2-l-L)$$

are to be simplified here and $L_n^\alpha(x)$ denotes the Laguerre polynomial.[8]

The first important property of sum (24) is the validity of the relations

$$\varphi_{ab}^{ilL}(x,y)=-\frac{d}{dx}\varphi_{a-1b}^{il-1L}(x,y)$$
$$=-z\frac{d}{dy}\varphi_{ab-1}^{ilL-1}(x,y) \qquad (25)$$

that follow from the properties of the Laguerre polynomials.[8] Then it is sufficient to investigate the $l=L=0$ case only. Employing the relation between the Laguerre polynomial with $l=0$ and Hermite polynomial[8] we obtain

$$\varphi_{ab}^{i00}(r^2,R^2)=\frac{(-1)^M}{\pi rR}\sum_{n+N=M}z^Np_i(n-a,N-b)$$
$$\times\frac{H_{2n+1}(r)H_{2N+1}(R)}{(2n+1)!(2N+1)!}. \qquad (26)$$

The second important observation is that the relations

$$n\frac{H_{n+1}(r)}{(n+1)!}=-\frac{H_{n+1}(r)}{(n+1)!}+2r\frac{H_n(r)}{n!}-2\frac{H_{n-1}(r)}{(n-1)!} \qquad (27)$$

enable us to lower the degree of the polynomial p_i in Eq. (26). In general, the summation (24) over n, N may thus be reduced by Eqs. (25) and (27) to four basic types of sums:

$$S_g^Q(x_1,x_2)=\sum_{l=0}^{Q}\frac{H_{2l+\alpha_g}(x_n)H_{2Q-2l+\beta_g}(x_2)}{(2l+\alpha_g)!(2Q-2l+\beta_g)!},$$
$$g=1,2,3,4, \qquad (28)$$
$$\alpha_1=\alpha_2=\beta_2=\beta_4=1,\quad \alpha_3=\alpha_4=\beta_1=\beta_3=0.$$

Application of the addition theorem for Hermite polynomials[8] — the last important step — leads to the evaluation of functions (28). For physical reasons (equal masses of nucleons) we put $D=1$ and have

$$S_g^Q(x_1,x_2)=\frac{2^{M_g/2-1}}{M_g!}\left[H_{M_g}\left(\frac{x_1+x_2}{\sqrt{2}}\right)\right.$$
$$\left.+(-1)^{\alpha_g}H_{M_g}\left(\frac{x_2-x_1}{\sqrt{2}}\right)\right], \qquad (29)$$
$$M_g=2Q+\alpha_g+\beta_g.$$

The generalization for $D\neq 1$ is straightforward.

We do not intend to overload this paper with formulas that follow immediately from the described method. Let us give only the simplest result ($F=n_1=l_1=l=L=\lambda=0$)

$$\psi_{n_2}(r,R)$$
$$=\delta_{l_20}2(rR)^{-1}\exp[-\tfrac{1}{2}(r^2+R^2)]\left\{\frac{(2n_2)!!}{\pi(2n_2+1)!!}\right\}^{1/2}$$
$$\times\{L_{n_2+1}^{-1/2}[\tfrac{1}{2}(r-R)^2]-L_{n_2+1}^{-1/2}[\tfrac{1}{2}(r+R)^2]\}. \qquad (30)$$

Using differentiation (25) we get from Eq. (30) the whole set of uncorrelated functions needed in ^{4}He.

B. Transition to the momentum variables

During all the preceding text we have supposed that the variables $\vec{r}_1$, $\vec{r}_2$ denote coordinates of the nucleons. Then the interpretation of RCM variables $\vec{r}, \vec{R}$ (for $D=1$) is evident. Nevertheless, other choices of RCM variables are very desirable. Since the Fourier-Bessel transformation changes only the phase factor of the oscillator wave function we may as well consider $\vec{r}_1, \vec{r}_2, \vec{r}, \vec{R}$ in Eqs. (1) and (3) to be particle and RCM momenta, without any changes in formulas (up to the overall phase factor).

A different situation arises when we perform only one transition from the coordinate into momentum space; single Fourier-Bessel transformation of Eq. (24) provides a new uncorrelated function of r (relative coordinate) and K (total momentum). The change of phase factor and $R=K$ variable in Eqs. (23)–(27) results in equivalent formulas with the different choice of z, $z=-D=-1$. The addition theorem provides the analog of Eqs. (28) and (29) in even more simple form:

$$\bar{S}_g^Q(x_1,x_2)=\sum_{l=0}^{Q}(-1)^{Q-l}\frac{H_{2l+\alpha_g}(x_1)H_{2Q-2l+\beta_g}(x_2)}{(2l+\alpha_g)!(2Q-2l+\beta_g)!},\quad g=1,2,3,4,$$
$$\bar{S}_{2t+1}^Q(x_1,x_2)=\frac{\mathrm{Re}(p^{M_g})}{(M_g)!},\quad \bar{S}_{2t+2}^Q(x_1,x_2)=\frac{\mathrm{Im}(p^{M_g})}{(M_g)!},\quad t=0,1, \tag{31}$$

where $p=2(x_1+ix_2)$.

Since the differentiation reproduces the set of functions (31), the results for $E_1>0$, $l>0$, $L>0$ may be derived readily using Eqs. (25) and (26).

As an example the uncorrelated function of the ^{4}He nucleus for $l=L=0$ is given here in final form

$$\psi_{n_2}(r,K)=\sum_{n+N=n_2}(n0,N0;0|00,n_20;0)_1R_{n0}(r)R_{N0}(K)(-1)^N=\frac{2\exp[-(r^2+K^2)/2]\,\mathrm{Im}[(K+ir)^{2n_2+2}]}{rK[(2n_2+1)!\pi]^{1/2}(n_2+1)}, \tag{32}$$

which is a remarkably simple analog of function (30).

C. Numerical aspects

The use of Eqs. (11)–(13) in numerical calculations should shorten the calculation time and increase precision, especially for $n_2 \gg n_1$. The last point may be demonstrated for $D=1$, $n_1=l_1=0$ by comparing both sides of Eq. (7) when $\alpha=\beta=0$, $m=n$. For $n=20$, eight significant digits are lost in Eq. (6) since $2^{-n}=10^{-6}$ and $\max\binom{n}{k}2^{-k}=6\times10^2$ for $k=k_0=[\frac{1}{3}(n+1)]=7$.

Let us finally touch on numerical questions connected with evaluation of the functions $\bar{S}_g^Q(x_1,x_2) \equiv \varphi_{M_g}(x_1,x_2)$ in Eq. (31). The simple recurrence relation

$$\varphi_{n+1}(x_1,x_2)=\frac{4}{n+1}\left[x_1\varphi_n(x_1,x_2)-\frac{x_1^2+x_2^2}{n}\varphi_{n-1}(x_1,x_2)\right] \tag{33}$$

may be used; it defines the functions $\bar{S}_1^Q=\varphi_{2Q+1}$, $\bar{S}_3^Q=\varphi_{2Q}$ for initial values

$$\varphi_0(x_1,x_2)=1,\quad \varphi_1(x_1,x_2)=2x_1$$

and the functions

$$\bar{S}_2^Q=\varphi_{2Q+2},\quad \bar{S}_4^Q=\varphi_{2Q+1}$$

for the initialization

$$\varphi_0(x_1,x_2)=0,\quad \varphi_1(x_1,x_2)=2x_2.$$

The proof makes use of the recurrence relations valid for Chebyshev polynomials,[8] since

$$\bar{S}_g^Q(x_1,x_2)=\frac{2^{M_g}}{(M_g)!}(x_1^2+x_2^2)^{M_g/2}T_{M_g}[x_1(x_1^2+x_2^2)^{-1/2}],\quad g=2t+1,\ t=0,1, \tag{34}$$
$$\bar{S}_g^Q(x_1,x_2)=\frac{2^{M_g}}{(M_g)!}(x_1^2+x_2^2)^{M_g/2}\frac{x_2}{(x_1^2+x_2^2)^{1/2}}U_{M_g-1}[x_1(x_1^2+x_2^2)^{-1/2}],\quad g=2t+2,\ t=0,1,$$

where $T_n(x)$ and $U_n(x)$ denote the Chebyshev polynomial of the first and second kind, respectively.

The numerical stability of relations (33) may be discussed in a standard way (c.f., Ref. 9) and proves to be entirely satisfactory. The absolute error Δ of the function calculated for large n diminishes as $1/n$. For low n it is bounded by $\exp[n_0+1-1/(2n_0+2)]$ where $p=(x_1^2+x_2^2)^{1/2} =\frac{1}{2}[n_0(n_0+1)]^{1/2}\exp[1-1/(2n_0+2)]$. For large p, the relative error Δ/φ is estimated by $1/\Gamma(p)$ and is negligible. The comparison of numerical results of the recurrent and direct calculation of the ^{4}He function (32) is given in Table I. The zero values (for n_2 odd) are well reproduced (12 digit arithmetic is used) by the recurrence relation, which confirms its stability.

We may conclude that the recurrence relation (33) represents an adequate tool in the numerical evaluation of the hole-hole and particle-hole uncorrelated wave function.

TABLE I. Numerical test of the recurrence relation for uncorrelated function. For $r=K$, the recurrence result ψ_r is compared with the exact value ψ_{ex} as given by Eq. (32). The absolute and relative difference are denoted by $\epsilon_A = |\psi_r - \psi_{ex}|$ and $\epsilon_R = \epsilon_A / |\psi_r + \psi_{ex}|$, respectively. Twelve digit precision is used.

r	n	ψ_{ex}	ϵ_A	ϵ_R
0.1	20	1.929×10^{-60}	4×10^{-72}	1.04×10^{-12}
	21	0	1.909×10^{-74}	1
	22	-3.725×10^{-67}	18×10^{-79}	2.42×10^{-12}
1	1	0	5.000×10^{-13}	1
	2	-1.011×10^{-1}	0	0
	4	4.410×10^{-3}	1×10^{-15}	1.13×10^{-13}
	20	7.167×10^{-21}	34×10^{-33}	2.37×10^{-12}
	21	0	7.273×10^{-33}	1
	22	-1.384×10^{-23}	6×10^{-35}	2.17×10^{-12}
	40	9.247×10^{-51}	63×10^{-63}	3.41×10^{-12}
	41	0	8.570×10^{-63}	1
	42	-5.059×10^{-54}	44×10^{-66}	4.34×10^{-12}
5	1	0	7.500×10^{-22}	1
	2	-2.384×10^{-9}	5×10^{-21}	1.05×10^{-12}
	4	6.504×10^{-8}	1×10^{-20}	7.69×10^{-14}
	20	2.461×10^{-3}	3×10^{-15}	6.09×10^{-13}
	21	0	4.773×10^{-14}	1
	22	-2.970×10^{-3}	0	0
	40	2.888×10^{-5}	0	0
	41	0	5.475×10^{-16}	1
	42	-9.874×10^{-6}	11×10^{-18}	5.57×10^{-13}

V. CONCLUSIONS

The new formula for Moshinsky brackets is to be used in practice whenever one of the energies is bounded by fixed value F. The summation in the well known formula Eq. (6) given by Trlifaj is substituted by the tabulated polynomial, e.g., for $F=2$ (i.e., in the ^{40}Ca nucleus), three polynomials of first and second degree [Eq. (10)] are needed. A few terms survive in the remaining sum (for ^{40}Ca, maximum is six terms); the calculation should be very quick. Moreover, loss of precision is reduced.

However, the main advantage of compact analytic formulas for MB (special cases of the general formula are given here for $F=0$ and 1) is to be found in the clear parameter dependence.

(1) It is possible to perform λ averaging in an explicit way. This is done here for the Pauli projector.

(2) The dependence of MB on oscillator quantum numbers n, N is such that analytic summation may be easily performed. Details are given of the method for direct Moshinsky transformation, without summation over MB and oscillator functions. In this way a very useful basis is constructed, instead of the harmonic oscillator one, that may be used not only in the Brueckner theory, but also in all shell model oriented calculations.

APPENDIX

The function W may be written also in the form of a double sum

$$W_{LD}^{\alpha\beta}(N,m)=\sum_{s=0}^{\gamma}(-1)^{\gamma-s}\binom{m}{\gamma-s}D^s \times\sum_{k=0}^{s}(\gamma-k)!\binom{N}{s-k}\binom{\beta}{k} \times\frac{\Gamma(\alpha+L+3/2)}{\Gamma(\alpha-k+L+3/2)}, \qquad \text{(A1)}$$

$$\gamma=\alpha+\beta$$

with a restricted number of terms $[\le\frac{1}{2}(n_1+l_1+1)(3n_1+l_1+2)]$. It reduces to a simple sum for one of the upper indices equal to zero:

$$W_{LD}^{\alpha 0}(N,m)=\alpha!\sum_{k=0}^{\alpha}(-1)^{\alpha-k}D^k\binom{N}{k}\binom{m}{\alpha-k}, \qquad \text{(A2)}$$

$$W_{LD}^{0\beta}(N,m)=W_{LD}^{\beta 0}(N+L+\tfrac{1}{2},m). \qquad \text{(A3)}$$

The proof of Eqs. (A1)-(A3) may be performed employing Eq. (9) and mathematical induction. The use of the consequence of Eq. (9),

$$W_{LD}^{\alpha\beta+1}(N,m) =D(\alpha-\beta+L+\tfrac{1}{2})W_{LD}^{\alpha\beta}(N,m)+W_{LD}^{\alpha+1\beta}(N,m), \qquad \text{(A4)}$$

and relation (A1) in the form

$$W_{LD}^{\alpha\beta}(N,m)=\sum_{k=0}^{\beta}\binom{\beta}{k}D^k\frac{\Gamma(\alpha+L+3/2)}{\Gamma(\alpha-k+L+3/2)} \times W_{LD}^{\alpha+\beta-k,0}(N,m)$$

simplifies the proof considerably when performed for growing β and arbitrary α in (A1).

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