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An Efficient Approach for the Calculation of Nuclear Overlap Integrals by Means of Binomial Coefficients and Its Application

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Abstract This paper examines the computational efficiency of the method of evaluating nuclear overlap integrals commonly encountered in nuclear reactions. As will be seen, the present formulation yields compact closed-form expressions which will make the calculation of nuclear overlap integrals easy. For practical applications, the computational technique used must be amenable to rapid evaluation and yield an acceptable degree of accuracy. Finally, the ratios $\frac{I_1(r)}{I_0(r)}$ for the non-Borromean two-nucleon halo systems are calculated by using new formulas which are important for the reaction analyses. The results of this calculation have been compared with those obtained according to one of the theoretical articles (Timofeyuk et al., Phys. Rev. C 68:021601(R), 2003). The same numerical results are presented for significant examples and they are briefly discussed.

Keywords Nuclear overlap integrals · Non-Borromean two-neutron halos · Single-nucleon overlap function · Auxiliary functions · Binomial coefficients

1 Introduction

It is well known that nuclear overlap integrals appear to be important parts of matrix elements within various approaches to nuclear reactions. Consider a non-relativistic composite bound system a, say, a nucleus, which can be divided into two subsystems (fragments) b and c. In fact, the overlap integral $I(\vec{r})$ is the projection of the wave function of a onto the $b+c$ channel. In this paper we study the numerical solution of a particular case of integrals that determine the Feyman diagram of Fig. 1 panels (a) and (b) in [1] for the virtual process $a \to b + c$ and is called nuclear overlap integral $I(\vec{r})$. This type of overlap integrals arises in the calculation of the cross sections determined by the asymptotics at large r corresponding to the $a \leftrightarrow b + c$ vertex. Although analytical expression of

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nuclear overlap integrals have not yet been sufficient so far, this function is of great importance in the various approaches of nuclear reactions as related to the Blokhintsev [1] technique since the non-Borromean two-neutron halos the effective local potential $V_{eff}(r)$ can be described explicitly in terms of this nuclear overlap integrals [2]. With this spirit in mind, an attempt is made in this paper to obtain general analytic expressions for nuclear overlap integrals. The theoretical efficient background of the presented paper is given in [1–10].

For the calculation of nuclear overlap integrals in [5] authors proposed the efficient formulas in special case $s = 3/2$. In [5], the nuclear overlap integrals have been expressed in terms of Error functions. In the present paper we propose analytical expression formulas in terms of binomial coefficients and A_k molecular auxiliary functions and E_k exponential integral functions, which make possible the fast and accurate evaluation of the nuclear overlap integrals for arbitrary values s.

The paper presents a numerical method of evaluation of the triangular diagram amplitude with constant vertices in a three body approach without the Coulomb interaction. The validity and reliability of the method is tested by applying it to lightest nuclei, for example the non-Borromean two-nucleon halo systems. The practical importance of $\frac{I_1(r)}{I_0(r)}$ ratios of the non-Borromean two-nucleon halo systems have been verified in [5] as "In the most extreme case of $S_{A-1}(1N) = S_A(2N)$, k_1 can be larger than k_2 by only 40% and the ratio $\frac{I_1(r)}{I_0(r)}$ decreases only slowly in the region between 5 and 10 fm of importance to reaction analyses (see Table 3)". This paper describes the derivation and explores the practical application of the results.

2 General Definition and Basic Formulas

The nuclear overlap integrals of simplest Feyman diagram for an $a \to b + c$ vertex is a triangle diagram of Fig. 1 in [1] which is defined as

$$I_1(s, k_1, k_2, r) = \frac{C}{r} \int_{k_1}^{\infty} \frac{e^{-kr}(k - k_1)^s}{k^2 - k_2^2} k dk, \tag{1}$$

where $s = 0, 3/2, 3, 9/2, \ldots$. See [1, 2] for exact definition of coefficients C, r, k_1 and k_2. We note that integral (1) is not the whole overlap function but only the part of it which leads to the anomalous asymptotics. One of the efficient method for the calculation nuclear overlap integral $I_1(r) = I_1(3/2, k_1, k_2, r)$ for special case $s = 3/2$ has been proposed by Timofeyuk et al. (see [5], (6)):

$$I_1(r) = -\left(1 - \frac{1}{2k_1 r}\right) \frac{C\sqrt{\pi} k_1}{r^{3/2}} e^{-k_1 r} + \frac{C\pi}{2r} \{(k_1 - k_2)^{3/2} e^{-kr} erfc[\sqrt{(k_1 - k_2)r}]$$
$$+ (k_1 + k_2)^{3/2} e^{kr} erfc[\sqrt{(k_1 + k_2)r}]\}. \tag{2}$$

Here $erfc(x)$ is error function defined by [22]

$$erfc(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt. \tag{3}$$

Also, in the article [5] the $V_{eff}(r)$ effective potential explicitly in terms nuclear overlap integrals are given as

$$V_{eff}(r) = -\frac{\hbar^2}{2\mu_1} c_{10} \sqrt{\frac{\pi}{k_1}} \frac{e^{-(k_1-k_2)r}}{r^{5/2}} \frac{1+\frac{5}{2k_1 r}}{1+\frac{I_1(r)}{I_0(r)}}, \tag{4}$$

where

$$I_0(r) \to C_0 \frac{e^{-k_2 r}}{r}. \tag{5}$$

See [5] for exact definition of coefficients r, c_{10} and μ. The practical importance of this work has been verified in [1, 5]. In article [5] the authors indicated that "The theoretical interpretation of the experimental data from these reactions relies on nuclear structure and reaction theories in which the single-particle state information enters through the one-nucleon overlap integrals. An important feature of these direct reaction mechanisms is that their amplitudes are primarily sensitive to the behavior of the one-nucleon overlaps at and beyond the nuclear surface". As can be seen from (4) and [1, 5], choice of reliable formulas for evaluation of $I_1(r)$ nuclear overlap integrals has the prime importance in the accurate calculation of the $V_{eff}(r)$ effective potential and other applications.

We note that (1) is not the whole overlap functions but approximation which reproduces the tail of the overlap function and to some extent its behavior near nuclear surface.

3 Series Relation for Nuclear Overlap Integrals Using Binomial Expansion Theorem

In order to express the nuclear overlap integral (1) in terms of auxiliary functions, we shall use the following well-known binomial expansion theorem (see [11–15]):

$$(x \pm y)^n = \sum_{m=0}^{\infty} (\pm 1)^m F_m(n) x^{n-m} y^m, \tag{6}$$

where $F_0(n) = 1$ and

$$F_m(n) = \begin{cases} \frac{n(n-1)\cdots(n-m+1)}{m!} & \text{for integer } n, \\ \frac{(-1)^m \Gamma(m-n)}{m!\Gamma(-n)} & \text{for noninteger } n. \end{cases} \tag{7}$$

We notice that for $m < 0$ the binomial coefficient $F_m(n)$ in (7) is zero and the positive values of integer n terms with negative factorials do not contribute to the summation. For fast calculations for the positive integer values of n, the binomial coefficients are stored in the memory of the computer. For the binomial coefficients, we use the following recurrence relation:

$$F_m(n) = F_m(n-1) + F_{m-1}(n-1). \tag{8}$$

In order to put these coefficients into or to get them back from the memory, the positions of certain coefficients $F_m(n)$ are determined by relation:

$$F(n,m) = n(n+1)/2 + m + 1. \tag{9}$$

Now we move on to the determination of expression for the nuclear overlap integrals in terms of binomial coefficients, and auxiliary functions. Taking (6) into account in (1) we obtain for the nuclear overlap integrals following simply structured formula:

- for integer values s:

$$I_1(s,k_1,k_2,r) = \frac{Ck_1^s}{r}\lim_{N\to\infty}\sum_{i=0}^{N}\sum_{j=0}^{s}(-1)^{i+j}F_i(-1)F_j(s)\left(\frac{k_2}{k_1}\right)^{2i} \times \begin{cases} A_{s-2i-j-1}(k_1r) & \text{for } s-2i-j-1\geq 0, \\ E_{|s-2i-j-1|}(k_1r) & \text{for } s-2i-j-1<0. \end{cases} \tag{10}$$

- for noninteger values s:

$$I_1(s,k_1,k_2,r) = \frac{Ck_1^s}{r}\lim_{N\to\infty,N'\to\infty}\sum_{i=0}^{N}\sum_{j=0}^{N'}(-1)^{i+j}F_i(-1)F_j(s)\left(\frac{k_2}{k_1}\right)^{2i} \times \begin{cases} A_{s-2i-j-1}(k_1r) & \text{for } s-2i-j-1\geq 0, \\ E_{|s-2i-j-1|}(k_1r) & \text{for } s-2i-j-1<0. \end{cases} \tag{11}$$

Here the indices N and N' are the upper limits of summations and

$$E_n(x) = \int_1^\infty t^{-n}e^{-xt}dt \tag{12}$$

are the well-known exponential integrals and $A_k(x)$ is the molecular auxiliary function [22, 23]. In order to avoid factorials, the formulas have been expressed in terms of binomial coefficients. For quick calculations, the binomial coefficients are stored in the memory of the computer. We note that the choice of reliable formulas for evaluation of these auxiliary functions has the prime importance in the accurate calculations. Several procedures for evaluating the exponential integral can be found in the literature [11–21]. For the calculation of auxiliary functions $A_k(x)$ defined by

$$A_k(x) = \int_1^\infty \mu^k e^{-x\mu}d\mu \tag{13}$$

the useful algorithm and efficient computer programs have been established in our works [15–19].

For those values of parameters for which the integral exists, the program Mathematica gives the following result

$$\begin{aligned} &I_1(s,k_1,k_2,r) \\ &= \frac{e^{-k_2r}\Gamma(s+1)}{2k_2}\{[k_1\Gamma(-s,(k_1-k_2)r)+(s+1)(k_1-k_2)\Gamma(-s-1,(k_1-k_2)r)] \\ &\quad\times(k_1-k_2)^s + e^{-2k_2r}(k_1+k_2)^s[k_1\Gamma(-s,(k_1+k_2)r) \\ &\quad+(s+1)(k_1+k_2)\Gamma(-s-1,(k_1+k_2)r)]\}. \end{aligned} \tag{14}$$

Note that this expression agrees with all numerical values given in the paper of (11).

4 Numerical Calculations and Discussion

In the paper we propose a new method of evaluation for the nuclear overlap integrals. Our main result contains analytical sums of simple binomial coefficients and auxiliary functions

Table 1 The comparative values of nuclear overlap integrals for $C = 1$, $N = 150$ and $N' = 300$

k_1	k_2	r	s	Equations (10) and (11)	[5] for (6)
0.7	0.5	3.5	1.5	1.3758028383E−03	1.3758060175E−03
1.5	0.8	6.3	1.5	1.1063510496E−07	1.1063851692E−07
1.69	1.38	4.3	1.5	4.4495451406E−06	4.4496587926E−06
1.69	1.38	1.4	1.5	1.6373963199E−02	1.6374010664E−02
1.72	1.09	3.4	1.5	2.9008435629E−05	2.9008778482E−05
1.72	1.09	7.3	1.5	3.1010152417E−09	3.1017161494E−09
1.72	1.09	10.7	1.5	2.5586654669E−12	2.5590383936E−12
2.7	1.6	3.7	1.5	2.4847295548E−07	2.4848195477E−07
2.7	1.6	3.7	3	1.3339835700E−07	
4.2	2.1	5.3	3	7.6855090394E−14	
5.4	4.2	8.5	3	5.5785001525E−25	
1.69	1.38	8.5	3	6.5434375633E−11	
1.69	1.38	8.5	4.5	1.9257839768E−11	
3.1	2.3	10.8	4.5	1.3788505642E−20	
5.31	3.23	4.3	4.5	9.8604926637E−14	
2.5	1.3	2.4	4.5	1.0445577314E−04	
6.2	2.1	3.2	4.5	9.0551547402E−12	
3.6	2.2	3.2	9	1.7248076605E−06	
6.6	4.2	5.3	9	3.9871305200E−19	
7.6	6.4	7.5	9	3.5563545104E−29	

Table 2 Convergence of derived expression (9) for $I_1(3, 4.2, 3.6, 1.2)$ as a function of summation limits N

N	Equation (10)
50	0.00309204192340231504378 4201
60	0.00309204192341112792703 6520
70	0.00309204192341133437505 4004
80	0.00309204192341133970298 4296
90	0.00309204192341133985079 8742
100	0.00309204192341133985513 6219
110	0.00309204192341133985526 9328
120	0.00309204192341133985527 3565
130	0.00309204192341133985527 3704
140	0.00309204192341133985527 3709
150	0.00309204192341133985527 3709

which must be evaluated efficiently and accurately. Table 1 shows that a short program written in Maple 8.0 international mathematical software gives accurate results for several comparative examples. To demonstrate the reliability of the method we compare our results with other calculations [5] and provide estimates for its range of applicability. The nuclear overlap integrals are computed using the formulas presented in [5] for $s = 3/2$ and our formulae ((10) and (11)). The tests clearly indicate that for $s > 3/2$ the formulas obtained

Table 3 Non-Borromean two-nucleon halo nuclei A, one-nucleon halo nuclei $A-1$, and their common $A-2$. The two- an done-nucleon thresholds $S_A(2N)$, $S_A(1N)$ and $S_{A-1}(1N)$ are also shown [5]

A	$A-1$	$A-2$	$S_A(2N)$ (MeV)	$S_A(1N)$ (MeV)	$S_{A-1}(1N)$ (MeV)
^{12}Be	^{11}Be($\frac{1}{2}^+$)	^{10}Be	3.670	3.170	0.500
^{12}Be	^{11}Be($\frac{1}{2}^-$)	^{10}Be	3.670	3.490	0.180
^{15}B	^{14}B(1^-)	^{13}B	3.740	3.510	0.230
^{9}C	^{8}B(g.s.)	^{7}Be	1.433	1.296	0.137
^{16}C	^{15}C($\frac{1}{2}^+$)	^{14}C	5.469	4.251	1.218
^{16}C	^{15}C($\frac{5}{2}^+$)	^{14}C	5.469	4.991	0.748

Table 4 The comparative values of ratios $\frac{I_1(r)}{I_0(r)}$ in the asymptotic region for $k_1=\sqrt{2}k_2$, $N=30$, $N'=200$ and $C_0/C=1\,fm^{3/2}$

k_2	r	Equation (11)	Equation (2)
0.6	5	7.1769E−03	7.1771E−03
0.5	5	9.7015E−03	9.7016E−03
0.5	10	8.2654E−04	8.2659E−04
0.4	9	2.0979E−03	2.0979E−03
0.4	6	7.8507E−03	7.8507E−03
0.3	7	7.5266E−03	7.5267E−03
0.3	10	2.5374E−03	2.5375E−03
0.2	6	1.7534E−02	1.7534E−02
0.2	9	6.2781E−03	6.2782E−03

yield significant accuracy for arbitrary values of integral parameters. Greater accuracy is easily attainable by the use of more terms of expansions (10) and (11).

Table 2 lists partial summations corresponding to progressively increasing upper summation limit (denoted N) for this expression. As can be seen from Table 2, (10) displays the most rapid convergence to the numerical result, with twenty five digits stable and correct by the hundred fiftieth terms in the infinite summation. For the numerical evaluation of $E_n(x)$ exponential integral and $A_n(x)$ molecular auxiliary function which occurs in the analytic expression of the nuclear overlap integrals, we used methods recently developed by [16–21].

The analytical relations for the nuclear overlap integrals derived in this paper are applied to the ratios $\frac{I_1(r)}{I_0(r)}$ of non-Borromean two-nucleon halo systems which have been measured in [5, 8] (see Table 3). The calculation results of the ratios $\frac{I_1(r)}{I_0(r)}$ of non-Borromean two-nucleon halo systems are presented in Table 4. As can be seen, our computational results are in good agreement with [5].

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