

W. Glöckle · H. Witała

# The Six-Nucleon Yakubovsky Equations for ${}^6\text{He}$

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**Abstract** The six-nucleon problem for the bound state is formulated in the Yakubovsky scheme. Hints for a numerical implementation are provided.

## 1 Introduction

There is a rich literature on  ${}^6\text{He}$  based on an effective  $\alpha - n - n$  3-body problem (1). Besides pair interactions also ad hoc 3-body forces are used. The Pauli principle is approximately incorporated by projecting out “Pauli forbidden states” for the neutrons inside the  $\alpha$ -particle wave function. While that approach catches presumably the halo structure of the two loosely bound neutrons clearly because of its strongly restricted ansatz it is not suited to probe modern nucleon–nucleon and three-nucleon forces, like the ones derived recently through effective field theory and based on chiral symmetry (2).

Nevertheless some approaches already exist which directly attack the 6-nucleon problem and beyond with realistic nuclear forces. We mention the No-Core Shell Model (NCSM) (3; 4; 5), the Greens Function Monte Carlo treatment (6), the Similarity Renormalisation Group (7), the Renormalisation Group evolution to low momentum interactions (8) and the coupled cluster (CC) theory (9). Further, the Nonsymmetrized Hyperspherical Harmonics approach (10) appears to be quite promising to deal with permutational-symmetry breaking terms in the Hamiltonian. In (3; 4; 5) chiral two-nucleon and three-nucleon forces were used and applied to  ${}^7\text{Li}$  with some underbinding. In (7) standard nuclear forces as well as forces based on chiral effective field theory are used and applied to light nuclei up to  ${}^6\text{Li}$ . In (8) the hyperspherical harmonics method is used for the Helium halo nucleus  ${}^6\text{He}$  and the CC approach for  ${}^8\text{He}$  both based on chiral nuclear forces. In

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ckle Institut für theoretische Physik II, Ruhr-Universität Bochum, 44780 Bochum, Germany  
Walter.Gloeckle@tp2.ruhr-uni-bochum.de · H. Witała M. Smoluchowski Institute of Physics,  
Jagiellonian University, 30059 Kraków, Poland witala@if.uj.edu.pl

(6) the AV18 nucleon–nucleon interaction and a Urbana three-nucleon force was used again leading to some underbinding, now for  ${}^6\text{He}$ . There is also the stochastic variational Monte Carlo method (11) which, however, still applied simplified forces.

The exploration of chiral forces goes on, also including explicitly the  $\Delta$ -degree of freedom (E. Epelbaum, Private communication), which calls for an increased effort to establish rigorous approaches beyond  $A = 4$ . The achievements in (3; 4; 5) and (6) demonstrate that a direct treatment of 6 nucleons is feasible on present day computers and therefore we felt that another approach, the exact formulation within the Yakubovsky equations, is timely. About 20 years ago an analogous step turned out to be very fruitful, namely the exact formulation of the  $\alpha$ -particle within the Yakubovsky scheme (12; 13). This pioneering study opened the way to a nowadays standard treatment (14; 15; 16; 17) and allows the inclusion of the most modern two- and three-nucleon forces and even first estimates of four-nucleon forces (18).

In Sect. 2 we apply the Yakubovsky equations (19) to the six-body problem using the basic notation for sub clusters (20). In Sect. 3 we add the identity of the nucleons which leads to a set of 5 coupled Yakubovsky equations related to 5 different sequential sub clusterings of 6 particles. In view of the expectation for the dominant structure of  ${}^6\text{He}$ , namely an  $\alpha$ -core and two loosely bound neutrons, we stop the sequential sub clustering with 3 fragments, though the additional step with two fragments could be easily performed.

In Sect. 4 and the Appendices we provide technicalities which we consider useful for a numerical performance. Finally we summarize in Sect. 5.

## 2 The Yakubovsky Approach to 6 Particles

We use the standard notation  $a_n$  to denote the various members of  $n$  fragments for a total of  $N$  particles. Here  $N = 6$  and  $a_2, a_3, a_4, a_5$  denote two-, three-, up to 5-body fragmentations. 5-body fragmentations necessarily have one pair left and thus  $a_5$  can be used to point to a specific pair.

$a_3 \subset a_2$  means that the three-body fragments  $a_3$  consist of sub clusters out of the two fragments in  $a_2$  or  $a_3 \supset a_4$  means that the sub clusters  $a_3$  when broken up lead to the sub clusters  $a_4$ .

The bound state  $\Psi$  obeys the homogeneous equation

$$\Psi = G_0 \sum_{a_5} V_{a_5} \Psi \quad (1)$$

where  $G_0$  is the 6-particle free Greens operator and  $V_{a_5}$  is a pair force. The first step is the summation of each pair force to infinite order. Defining

$$\psi_{a_5} \equiv G_0 V_{a_5} \Psi \quad (2)$$

one obtains like for 3 particles

$$\psi_{a_5} = G_0 t_{a_5} \sum_{b_5} \overline{\delta_{a_5 b_5}} \psi_{b_5} \quad (3)$$

where  $t_{a_5}$  is a two-body t-operator obeying the Lippmann Schwinger equation

$$t_{a_5} = V_{a_5} + V_{a_5} G_0 t_{a_5} \quad (4)$$

and  $\overline{\delta_{a_5 b_5}} \equiv 1 - \delta_{a_5 b_5}$ .

Next one defines new components

$$\psi_{a_5 a_4} \equiv G_0 t_{a_5} \sum_{b_5 \subset a_4} \overline{\delta_{a_5 b_5}} \psi_{b_5} \quad (5)$$

where all pairs  $a_5, b_5$  are sub clusters of the fragments in  $a_4$ . Clearly

$$\psi_{a_5} = \sum_{a_4 \supset a_5} \psi_{a_5 a_4} \quad (6)$$

That relation (6) is used to obtain a closed set of equations for  $\psi_{a_5 a_4}$ :

$$\psi_{a_5 a_4} = G_0 t_{a_5} \sum_{b_5 \subset a_4} \overline{\delta_{a_5 b_5}} \sum_{b_4 \supset b_5} \psi_{b_5 b_4} \quad (7)$$

One separates now the components  $\psi_{a_5 a_4}$  for a given  $a_4$  from the rest:

$$\psi_{a_5 a_4} - G_0 t_{a_5} \sum_{b_5 \subset a_4} \overline{\delta_{a_5 b_5}} \psi_{b_5 a_4} = G_0 t_{a_5} \sum_{b_5 \subset a_4} \overline{\delta_{a_5 b_5}} \sum_{b_4 \supset b_5} \overline{\delta_{a_4 b_4}} \psi_{b_5 b_4} \quad (8)$$

Let us define for a fixed  $a_4$  the column vectors  $\psi^{a_4}$  and  $\psi^{(a_4)}$  with the components

$$(\psi^{a_4})_{a_5} \equiv \psi_{a_5 a_4} \quad (9)$$

and

$$(\psi^{(a_4)})_{b_5} \equiv \sum_{b_4 \supset b_5} \overline{\delta_{a_4 b_4}} \psi_{b_5 b_4} \quad (10)$$

Then introducing the matrix  $C^{a_4}$  with the elements  $C_{a_5 b_5}^{a_4} \equiv t_{a_5} \overline{\delta_{a_5 b_5}}$  Eq. (8) reads

$$(1 - G_0 C^{a_4}) \psi^{a_4} = G_0 C^{a_4} \psi^{(a_4)} \quad (11)$$

or

$$\psi^{a_4} = (1 - G_0 C^{a_4})^{-1} G_0 C^{a_4} \psi^{(a_4)} \equiv G_0 T^{a_4} \psi^{(a_4)} \quad (12)$$

Apparently  $T^{a_4}$  obeys

$$T^{a_4} = C^{a_4} + C^{a_4} G_0 T^{a_4} \quad (13)$$

In explicite notation (12) and (13) read

$$\psi_{a_5 a_4} = G_0 \sum_{b_5 \subset a_4} T_{a_5 b_5}^{a_4} \psi_{b_5}^{(a_4)} = G_0 \sum_{b_5 \subset a_4} T_{a_5 b_5}^{a_4} \sum_{b_4 \supset b_5} \overline{\delta_{a_4 b_4}} \psi_{b_5 b_4} \quad (14)$$

$$T_{a_5 b_5}^{a_4} = t_{a_5} \overline{\delta_{a_5 b_5}} + \sum_{c_5 \subset a_4} t_{a_5} \overline{\delta_{a_5 c_5}} G_0 T_{c_5 b_5}^{a_4} \quad (15)$$

Note, there are two types of T-matrices. For  $a_4$  of the type 123,4,5,6  $T_{a_5 b_5}^{a_4}$  is a  $3 \times 3$  matrix and for  $a_4$  of the type 12,34,5,6  $T_{a_5 b_5}^{a_4}$  is a  $2 \times 2$  matrix.

Next we further decompose the right-hand side of (14) according to 3-body fragments  $a_3$ :

$$\psi_{a_5 a_4}^{a_3} \equiv \sum_{b_5 \subset a_4} G_0 T_{a_5 b_5}^{a_4} \sum_{b_4 \supset b_5, b_4 \subset a_3} \overline{\delta_{a_4 b_4}} \psi_{b_5 b_4} \quad (16)$$

and again

$$\psi_{a_5 a_4} = \sum_{a_3 \supset a_4} \psi_{a_5 a_4}^{a_3} \quad (17)$$

is an obvious consequence.

Using again (17) Eq. (16) can be rewritten as

$$\psi_{a_5 a_4}^{a_3} = \sum_{b_5 \subset a_4} G_0 T_{a_5 b_5}^{a_4} \sum_{b_4 \supset b_5, b_4 \subset a_3} \overline{\delta_{a_4 b_4}} \sum_{b_3 \supset b_4} \psi_{b_5 b_4}^{b_3} \quad (18)$$

Analogous to (8) one separates  $b_3 = a_3$  from  $b_3 \neq a_3$  and gets

$$\psi_{a_5 a_4}^{a_3} - G_0 \sum_{b_5 \subset a_4} T_{a_5 b_5}^{a_4} \sum_{b_4 \supset b_5, b_4 \subset a_3} \overline{\delta_{a_4 b_4}} \psi_{b_5 b_4}^{a_3} = G_0 \sum_{b_5 \subset a_4} T_{a_5 b_5}^{a_4} \sum_{b_4 \supset b_5, b_4 \subset a_3} \overline{\delta_{a_4 b_4}} \psi_{b_5 b_4}^{(a_3)} \quad (19)$$

where we defined

$$\psi_{b_5 b_4}^{(a_3)} \equiv \sum_{b_3 \supset b_4} \overline{\delta_{a_3 b_3}} \psi_{b_5 b_4}^{b_3} \quad (20)$$

Using a matrix notation it is easily seen that (19) leads to

$$\psi_{a_5 a_4}^{a_3} = G_0 \sum_{b_4 \subset a_3} \sum_{b_5 \subset b_4} D_{a_5, a_4; b_5 b_4}^{a_3} \psi_{b_5 b_4}^{(a_3)} \quad (21)$$

where  $D_{a_5, a_4; b_5 b_4}^{a_3}$  obeys

$$D_{a_5, a_4; b_5 b_4}^{a_3} = T_{a_5 b_5}^{a_4} \overline{\delta_{a_4 b_4}} + \sum_{c_4 \subset a_3} \sum_{c_5 \subset a_4} T_{a_5 c_5}^{a_4} \overline{\delta_{a_4 c_4}} G_0 D_{c_5, c_4; b_5 b_4}^{a_3} \quad (22)$$

Note for  $a_3 = 1234, 5, 6$  there are 18 pairs of  $a_5, a_4$ , for  $a_3 = 123, 45, 6$  there are 9 pairs of  $a_5, a_4$  and for  $a_3 = 12, 34, 56$  there are 6 pairs of  $a_5, a_4$ . This defines the dimensions of the different D-matrices. In the following the single nucleons in  $a_n$  will no longer be displayed.

### 3 Implementation of the Identity of the Nucleons

We start from (14) choosing the case  $a_5 = 12$  and  $a_4 = 12, 34$  and obtain

$$\psi_{12;12,34} = G_0 T_{12,12}^{12,34} \psi_{12}^{(12,34)} + G_0 T_{12,34}^{12,34} \psi_{34}^{(12,34)} \quad (23)$$

which according to (10) is

$$\begin{aligned} \psi_{12;12,34} = & G_0 T_{12,12}^{12,34} (\psi_{12,123} + \psi_{12,124} + \psi_{12,125} + \psi_{12,126} \\ & + \psi_{12,12,35} + \psi_{12,12,36} + \psi_{12,12,45} + \psi_{12,12,46} + \psi_{12,12,56}) \\ & + G_0 T_{12,34}^{12,34} (\psi_{34,134} + \psi_{34,234} + \psi_{34,345} + \psi_{34,346} \\ & + \psi_{34,34,15} + \psi_{34,34,16} + \psi_{34,34,25} + \psi_{34,34,26} + \psi_{34,34,56}) \end{aligned} \quad (24)$$

It is easily seen, going back to the definitions (2) and (5) together with the antisymmetry requirement for the total state  $\Psi$  that

$$\begin{aligned} \psi_{34,134} + \psi_{34,234} + \psi_{34,345} + \psi_{34,346} + \psi_{34,34,15} + \psi_{34,34,16} + \psi_{34,34,25} \\ + \psi_{34,34,26} + \psi_{34,34,56} = P_{13} P_{24} (\psi_{12,123} + \psi_{12,124} + \psi_{12,125} + \psi_{12,126} \\ + \psi_{12,12,35} + \psi_{12,12,36} + \psi_{12,12,45} + \psi_{12,12,46} + \psi_{12,12,56}) \end{aligned} \quad (25)$$

Therefore (24) turns into

$$\begin{aligned} \psi_{12;12,34} = & G_0 (T_{12,12}^{12,34} + T_{12,34}^{12,34} P_{13} P_{24}) (\psi_{12,123} + \psi_{12,124} + \psi_{12,125} + \psi_{12,126} \\ & + \psi_{12,12,35} + \psi_{12,12,36} + \psi_{12,12,45} + \psi_{12,12,46} + \psi_{12,12,56}) \end{aligned} \quad (26)$$

The coupled equations (15) written out for  $a_4 = 12, 34$  and  $a_5$  or  $b_5$  equal to 12 or 34 yield when acting with  $\tilde{P} \equiv P_{13} P_{24}$  from both sides

$$\begin{aligned} \tilde{P} T_{12,12}^{12,34} \tilde{P} &= T_{34,34}^{12,34} \\ \tilde{P} T_{12,34}^{12,34} \tilde{P} &= T_{34,12}^{12,34} \end{aligned} \quad (27)$$

Then defining

$$T^{12,34} \equiv T_{12,12}^{12,34} + T_{12,34}^{12,34} \tilde{P} \quad (28)$$

it follows that  $T^{12,34}$  obeys

$$T^{12,34} = t_{12} \tilde{P} + t_{12} G_0 \tilde{P} T^{12,34} \quad (29)$$

Therefore (26) simplifies to

$$\begin{aligned} \psi_{12;12,34} = & G_0 T^{12,34} (\psi_{12,123} + \psi_{12,124} + \psi_{12,125} + \psi_{12,126} + \psi_{12,12,35} \\ & + \psi_{12,12,36} + \psi_{12,12,45} + \psi_{12,12,46} + \psi_{12,12,56}) \end{aligned} \quad (30)$$

Starting again from (14) but now for  $a_5 = 12$  and  $a_4 = 123$  one obtains

$$\begin{aligned}
\psi_{12,123} &= G_0 T_{12,12}^{123} \psi_{12}^{(123)} + G_0 T_{12,23}^{123} \psi_{23}^{(123)} + G_0 T_{12,31}^{123} \psi_{31}^{(123)} \\
&= G_0 T_{12,12}^{123} (\psi_{12,124} + \psi_{12,125} + \psi_{12,126} \\
&\quad + \psi_{12,12,34} + \psi_{12,12,35} + \psi_{12,12,36} + \psi_{12,12,45} + \psi_{12,12,46} + \psi_{12,12,56}) \\
&\quad + G_0 T_{12,23}^{123} (\psi_{23,234} + \psi_{23,235} + \psi_{23,236} \\
&\quad + \psi_{23,23,14} + \psi_{23,23,15} + \psi_{23,23,16} + \psi_{23,23,45} + \psi_{23,23,46} + \psi_{23,23,56}) \\
&\quad + G_0 T_{12,31}^{123} (\psi_{31,314} + \psi_{31,315} + \psi_{31,316} \\
&\quad + \psi_{31,31,24} + \psi_{31,31,25} + \psi_{31,31,26} + \psi_{31,31,45} + \psi_{31,31,46} + \psi_{31,31,56}) \\
&= G_0 (T_{12,12}^{123} + T_{12,23}^{123} P_{12} P_{23} + T_{12,31}^{123} P_{13} P_{23}) (\psi_{12,124} + \psi_{12,125} + \psi_{12,126} \\
&\quad + \psi_{12,12,34} + \psi_{12,12,35} + \psi_{12,12,36} + \psi_{12,12,45} + \psi_{12,12,46} + \psi_{12,12,56})
\end{aligned}$$

where we used permutation properties similar as in (25).

The corresponding coupled sets (15) for  $a_4 = 123$  and using relations like

$$P_{13} P_{23} t_{23} P_{23} P_{13} = t_{12}$$

reveals that

$$T^{123} \equiv T_{12,12}^{123} + T_{12,23}^{123} P_{12} P_{23} + T_{12,31}^{123} P_{13} P_{23} \quad (32)$$

obeys the equation

$$T^{123} = t_{12} P + t_{12} P G_0 T^{123} \quad (33)$$

where  $P \equiv P_{12} P_{23} + P_{13} P_{23}$ .

Then (31) simplifies to

$$\begin{aligned}
\psi_{12,123} &= G_0 T^{123} (\psi_{12,124} + \psi_{12,125} + \psi_{12,126} + \psi_{12,12,34} + \psi_{12,12,35} + \psi_{12,12,36} \\
&\quad + \psi_{12,12,45} + \psi_{12,12,46} + \psi_{12,12,56})
\end{aligned} \quad (34)$$

The next step is to decompose  $\psi_{12,123}$  according to (16). For  $a_5 = 12, a_4 = 123$  the possible  $a_3$ 's are:  $1234 - 1235 - 1236 - 123,45 - 123,46 - 123,56$ .

Lets begin with

$$\begin{aligned}
\psi_{12,123}^{1234} &\equiv G_0 T_{12,12}^{123} (\psi_{12,124} + \psi_{12,12,34}) + G_0 T_{12,23}^{123} (\psi_{23,234} + \psi_{23,23,14}) \\
&\quad + G_0 T_{12,31}^{123} (\psi_{31,134} + \psi_{31,31,24})
\end{aligned} \quad (35)$$

Since

$$\begin{aligned}
\psi_{23,234} + \psi_{23,23,14} &= P_{12} P_{23} (\psi_{12,124} + \psi_{12,12,34}) \\
\psi_{31,134} + \psi_{31,31,24} &= P_{13} P_{23} (\psi_{12,124} + \psi_{12,12,34})
\end{aligned} \quad (36)$$

(35) simplifies according to (33) to

$$\psi_{12,123}^{1234} = G_0 T^{123} (\psi_{12,124} + \psi_{12,12,34}) \quad (37)$$

Similarly

$$\begin{aligned}\psi_{12,123}^{1235} &= G_0 T^{123} (\psi_{12,125} + \psi_{12,12,35}) \\ \psi_{12,123}^{1236} &= G_0 T^{123} (\psi_{12,126} + \psi_{12,12,36})\end{aligned}\quad (38)$$

Again using symmetry properties one gets

$$\psi_{12,123}^{123,45} = G_0 T^{123} \psi_{12,12,45} \quad (39)$$

$$\psi_{12,123}^{123,46} = G_0 T^{123} \psi_{12,12,46} \quad (40)$$

$$\psi_{12,123}^{123,56} = G_0 T^{123} \psi_{12,12,56} \quad (41)$$

All summed up

$$\psi_{12,123} = \psi_{12,123}^{1234} + \psi_{12,123}^{1235} + \psi_{12,123}^{1236} + \psi_{12,123}^{123,45} + \psi_{12,123}^{123,46} + \psi_{12,123}^{123,56} \quad (42)$$

agrees with (34).

Next we decompose (14) according to (16) for  $a_5 = 12, a_4 = 12, 34$ . The possible  $a_3$ 's are:  $1234 - 125, 34 - 126, 34 - 12, 345 - 12, 346 - 12, 34, 56$ , which are now regarded in turn.

$$\psi_{12,12,34}^{1234} = G_0 T_{12,12}^{12,34} (\psi_{12,123} + \psi_{12,124}) + G_0 T_{12,34}^{12,34} (\psi_{34,234} + \psi_{34,134}) \quad (43)$$

Since

$$P_{13}P_{24}(\psi_{12,123} + \psi_{12,124}) = \psi_{34,234} + \psi_{34,134} \quad (44)$$

one can use (28) and gets

$$\begin{aligned}\psi_{12,12,34}^{1234} &= G_0 (T_{12,12}^{12,34} + T_{12,34}^{12,34} P_{13}P_{24}) (\psi_{12,123} + \psi_{12,124}) \\ &= G_0 T^{12,34} (\psi_{12,123} + \psi_{12,124})\end{aligned}\quad (45)$$

Next

$$\begin{aligned}\psi_{12,12,34}^{125,34} &= G_0 T_{12,12}^{12,34} \psi_{12,125} + G_0 T_{12,34}^{12,34} (\psi_{34,15,34} + \psi_{34,25,34}) \\ \psi_{12,12,34}^{345,12} &= G_0 T_{12,12}^{12,34} (\psi_{12,12,35} + \psi_{12,12,45}) + G_0 T_{12,34}^{12,34} \psi_{34,345}\end{aligned}\quad (46)$$

The two amplitudes  $\psi_{12,12,34}^{125,34}$  and  $\psi_{12,12,34}^{345,12}$  cannot be related by permutations, but their sum can be used

$$\begin{aligned}\psi_{12,12,34}^{125,34} + \psi_{12,12,34}^{345,12} &= G_0 T_{12,12}^{12,34} (\psi_{12,125} + \psi_{12,12,35} + \psi_{12,12,45}) \\ &\quad + G_0 T_{12,34}^{12,34} (\psi_{34,15,34} + \psi_{34,25,34} + \psi_{34,345})\end{aligned}\quad (47)$$

in the sense

$$P_{13}P_{24}(\psi_{12,125} + \psi_{12,12,35} + \psi_{12,12,45}) = \psi_{34,15,34} + \psi_{34,25,34} + \psi_{34,345} \quad (48)$$

This leads to

$$\psi_{12,12,34}^{125,34} + \psi_{12,12,34}^{345,12} = G_0 T^{12,34} (\psi_{12,125} + \psi_{12,12,35} + \psi_{12,12,45}) \quad (49)$$

Similarly

$$\psi_{12;12,34}^{126,34} + \psi_{12;12,34}^{346,12} = G_0 T^{12,34} (\psi_{12,126} + \psi_{12;12,36} + \psi_{12;12,46}) \quad (50)$$

and finally

$$\psi_{12;12,34}^{12,34,56} = G_0 T_{12,12}^{12,34} \psi_{12;12,56} + G_0 T_{12,34}^{12,34} \psi_{34;34,56} = G_0 T^{12,34} \psi_{12;12,56} \quad (51)$$

Thus, Eqs. (45), (49)–(51), summarizes to

$$\psi_{12;12,34} = \psi_{12;12,34}^{1234} + \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} + \psi_{12;12,34}^{126,34} + \psi_{12;12,34}^{346,12} + \psi_{12;12,34}^{12,34,56} \quad (52)$$

which when written out agrees with (30).

The two amplitudes  $\psi_{12,123}^{1234}$  and  $\psi_{12;12,34}^{1234}$  expressed in (37) and (45) are connected to each other as shown now. The expression (42) can easily be converted to  $\psi_{12,124}$  and using in addition (52) one finds

$$\begin{aligned} \psi_{12,123}^{1234} - G_0 T^{123} (\psi_{12,124}^{1234} + \psi_{12;12,34}^{1234}) &= G_0 T^{123} \left( \psi_{12,124}^{1245} + \psi_{12,124}^{1246} + \psi_{12,124}^{124,35} + \psi_{12,124}^{124,36} + \psi_{12,124}^{124,56} \right. \\ &\quad \left. + \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} + \psi_{12;12,34}^{126,34} + \psi_{12;12,34}^{346,12} + \psi_{12;12,34}^{12,34,56} \right) \quad (53) \end{aligned}$$

Correspondingly (45) yields

$$\begin{aligned} \psi_{12;12,34}^{1234} - G_0 T^{12,34} (\psi_{12,123}^{1234} + \psi_{12,124}^{1234}) &= G_0 T^{12,34} \left( \psi_{12,123}^{1235} + \psi_{12,123}^{123,45} + \psi_{12,123}^{1236} + \psi_{12,123}^{123,46} + \psi_{12,123}^{123,56} \right. \\ &\quad \left. + \psi_{12,124}^{1245} + \psi_{12,124}^{124,35} + \psi_{12,124}^{1246} + \psi_{12,124}^{124,36} + \psi_{12,124}^{124,56} \right) \quad (54) \end{aligned}$$

With  $\psi_{12,124}^{1234} = -P_{34} \psi_{12,123}^{1234}$  we can put (53) and (54) into a matrix form:

$$\begin{aligned} &\begin{pmatrix} \psi_{12,123}^{1234} \\ \psi_{12;12,34}^{1234} \end{pmatrix} - G_0 \begin{pmatrix} -T^{123} P_{34} & T^{123} \\ T^{12,34} (1 - P_{34}) & 0 \end{pmatrix} \begin{pmatrix} \psi_{12,123}^{1234} \\ \psi_{12;12,34}^{1234} \end{pmatrix} \\ &= G_0 \begin{pmatrix} T^{123} \left( \psi_{12,124}^{1245} + \psi_{12,124}^{1246} + \psi_{12,124}^{124,35} + \psi_{12,124}^{124,36} + \psi_{12,124}^{124,56} + \psi_{12;12,34}^{125,34} \right. \right. \\ &\quad \left. \left. + \psi_{12;12,34}^{345,12} + \psi_{12;12,34}^{126,34} + \psi_{12;12,34}^{346,12} + \psi_{12;12,34}^{12,34,56} \right) \\ T^{12,34} \left( \psi_{12,123}^{1235} + \psi_{12,123}^{123,45} + \psi_{12,123}^{1236} + \psi_{12,123}^{123,46} + \psi_{12,123}^{123,56} + \psi_{12,124}^{1245} \right. \\ &\quad \left. + \psi_{12,124}^{124,35} + \psi_{12,124}^{1246} + \psi_{12,124}^{124,36} + \psi_{12,124}^{124,56} \right) \end{pmatrix} \quad (55) \end{aligned}$$

Since

$$\begin{aligned} \psi_{12,124}^{1245} &= -P_{34} \psi_{12,123}^{1235} \\ \psi_{12,124}^{124,35} &= -P_{34} \psi_{12,123}^{123,45} \end{aligned} \quad (56)$$



the right-hand side of (55) can be factored and (55) achieves the form

$$\begin{pmatrix} \psi_{12,123}^{1234} \\ \psi_{12,12,34}^{1234} \end{pmatrix} - G_0 \begin{pmatrix} -T^{123}P_{34} & T^{123} \\ T^{12,34}(1-P_{34}) & 0 \end{pmatrix} \begin{pmatrix} \psi_{12,123}^{1234} \\ \psi_{12,12,34}^{1234} \end{pmatrix} \\ = G_0 \begin{pmatrix} T^{123}(-P_{34}) & T^{123} \\ T^{12,34}(1-P_{34}) & 0 \end{pmatrix} \begin{pmatrix} \psi_{12,123}^{1235} + \psi_{12,123}^{123,45} + \psi_{12,123}^{1236} \\ + \psi_{12,123}^{123,46} + \psi_{12,123}^{123,56} \\ \psi_{12,12,34}^{125,34} + \psi_{12,12,34}^{345,12} + \psi_{12,12,34}^{126,34} \\ + \psi_{12,12,34}^{346,12} + \psi_{12,12,34}^{12,34,56} \end{pmatrix} \quad (57)$$

The right-hand side can be reduced applying permutations and one obtains

$$\begin{pmatrix} \psi_{12,123}^{1234} \\ \psi_{12,12,34}^{1234} \end{pmatrix} - G_0 \begin{pmatrix} -T^{123}P_{34} & T^{123} \\ T^{12,34}(1-P_{34}) & 0 \end{pmatrix} \begin{pmatrix} \psi_{12,123}^{1234} \\ \psi_{12,12,34}^{1234} \end{pmatrix} = G_0 \\ \begin{pmatrix} T^{123}(-P_{34}) & T^{123} \\ T^{12,34}(1-P_{34}) & 0 \end{pmatrix} \begin{pmatrix} -(P_{45}+P_{46})\psi_{12,123}^{1234} + (1-P_{56}-P_{46})\psi_{12,123}^{123,45} \\ (1-P_{56})(\psi_{12,12,34}^{125,34} + \psi_{12,12,34}^{345,12} + \psi_{12,12,34}^{12,34,56}) \end{pmatrix} \quad (58)$$

which can be put into the form  $\begin{pmatrix} \psi_{12,123}^{1234} \\ \psi_{12,12,34}^{1234} \end{pmatrix}$  with the result

$$\begin{pmatrix} \psi_{12,123}^{1234} \\ \psi_{12,12,34}^{1234} \end{pmatrix} \equiv G_0 \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \begin{pmatrix} -(P_{45}+P_{46})\psi_{12,123}^{1234} + (1-P_{56}-P_{46})\psi_{12,123}^{123,45} \\ (1-P_{56})(\psi_{12,12,34}^{125,34} + \psi_{12,12,34}^{345,12} + \psi_{12,12,34}^{12,34,56}) \end{pmatrix} \quad (59)$$

where the matrix  $D$  obeys

$$\begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} = \begin{pmatrix} -T^{123}P_{34} & T^{123} \\ T^{12,34}(1-P_{34}) & 0 \end{pmatrix} + \begin{pmatrix} -T^{123}P_{34} & T^{123} \\ T^{12,34}(1-P_{34}) & 0 \end{pmatrix} G_0 \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \quad (60)$$

For the numerical treatment, however, we consider the structure (58) to be more advantageous.

The right-hand side of (58) contains new amplitudes. After adequate permutation of (52) one obtains from (39)

$$\psi_{12,123}^{123,45} = G_0 T^{123} \left( \psi_{12,12,45}^{1245} + \psi_{12,12,45}^{123,45} + \psi_{12,12,45}^{345,12} + \psi_{12,12,45}^{456,12} + \psi_{12,12,45}^{126,45} + \psi_{12,12,45}^{12,45,36} \right) \quad (61)$$

or

$$\psi_{12,123}^{123,45} - G_0 T^{123} \left( -(1-P_{36})P_{53} \left( \psi_{12,12,34}^{125,34} + \psi_{12,12,34}^{345,12} \right) \right) = G_0 T^{123} \left( -P_{35} \psi_{12,12,34}^{1234} + \psi_{12,12,45}^{12,45,36} \right) \quad (62)$$

Further (49) yields inserting the decomposition of the right-hand side related to (42) and (52) yields

$$\begin{aligned} \psi_{12,12,34}^{125,34} + \psi_{12,12,34}^{345,12} &= G_0 T^{12,34} \left( \psi_{12,125}^{1235} + \psi_{12,125}^{1245} + \psi_{12,125}^{125,34} \right. \\ &\quad + \psi_{12,125}^{1256} + \psi_{12,125}^{125,36} + \psi_{12,125}^{125,46} + \psi_{12,12,35}^{1235} + \psi_{12,12,35}^{124,35} + \psi_{12,12,35}^{345,12} \\ &\quad + \psi_{12,12,35}^{356,12} + \psi_{12,12,35}^{126,35} + \psi_{12,12,35}^{12,56,34} + \psi_{12,12,45}^{1245} + \psi_{12,12,45}^{123,45} + \psi_{12,12,45}^{345,12} \\ &\quad \left. + \psi_{12,12,45}^{456,12} + \psi_{12,12,45}^{126,45} + \psi_{12,12,45}^{12,34,56} \right) \quad (63) \end{aligned}$$

Here quite a few amplitudes can be related to previous ones by permutations leading to:

$$\begin{aligned} & \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} - G_0 T^{12,34} (P_{35} P_{56} - P_{35} - P_{46} - P_{45}) \left( \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} \right) \\ &= G_0 T^{12,34} \left( (1 - P_{36} - P_{34} - P_{46}) P_{34} P_{35} \psi_{12;12,34}^{1234} + (1 - P_{34}) P_{46} P_{35} \psi_{12;12,34}^{123,45} \right. \\ & \quad \left. - (P_{45} + P_{35}) \psi_{12;12,34}^{1234} - P_{35} \psi_{12;12,34}^{12,34,56} \right) \end{aligned} \quad (64)$$

Finally we regard  $\psi_{12;12,34}^{12,34,56}$ , which after (51) and suitable permutations of (52) turns into

$$\begin{aligned} & \psi_{12;12,34}^{12,34,56} - G_0 T^{12,34} P_{35} P_{46} \psi_{12;12,34}^{12,34,56} \\ &= G_0 T^{12,34} \left( P_{35} P_{46} \psi_{12;12,34}^{1234} + (1 - P_{34}) P_{35} P_{46} \left( \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} \right) \right) \end{aligned} \quad (65)$$

where we used

$$\psi_{12;12,56}^{12,56,34} = G_0 T^{12,56} \psi_{12;12,34} = P_{35} P_{46} G_0 T^{12,34} \psi_{12;12,56} = P_{35} P_{46} \psi_{12;12,34}^{12,34,56} \quad (66)$$

Thus we end up with 5 independent amplitudes:  $\psi_{12;12,34}^{1234}$ ,  $\psi_{12;12,34}^{1234}$ ,  $\psi_{12;12,34}^{123,45}$ ,  $\psi_{12;12,34}^{125,34}$  +  $\psi_{12;12,34}^{345,12}$ , and  $\psi_{12;12,34}^{12,34,56}$ , coupled in the equations

$$\begin{aligned} & \begin{pmatrix} \psi_{12;12,34}^{1234} \\ \psi_{12;12,34}^{1234} \end{pmatrix} - G_0 \begin{pmatrix} -T^{123} P_{34} & T^{123} \\ T^{12,34} (1 - P_{34}) & 0 \end{pmatrix} \begin{pmatrix} \psi_{12;12,34}^{1234} \\ \psi_{12;12,34}^{1234} \end{pmatrix} = G_0 \\ & \begin{pmatrix} T^{123} (-P_{34}) & T^{123} \\ T^{12,34} (1 - P_{34}) & 0 \end{pmatrix} \begin{pmatrix} -(P_{45} + P_{46}) \psi_{12;12,34}^{1234} + (1 - P_{56} - P_{46}) \psi_{12;12,34}^{123,45} \\ (1 - P_{56}) \left( \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} \right) + \psi_{12;12,34}^{12,34,56} \end{pmatrix} \\ & \psi_{12;12,34}^{123,45} - G_0 T^{123} \left( -(1 - P_{36}) P_{53} \left( \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} \right) \right) \\ &= -G_0 T^{123} P_{35} \left( \psi_{12;12,34}^{1234} + \psi_{12;12,34}^{12,34,56} \right) \end{aligned} \quad (68)$$

$$\begin{aligned} & \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} - G_0 T^{12,34} (P_{35} P_{56} - P_{35} - P_{46} - P_{45}) \left( \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} \right) \\ &= G_0 T^{12,34} \left( (1 - P_{36} - P_{34} - P_{46}) P_{34} P_{35} \psi_{12;12,34}^{1234} + (1 - P_{34}) P_{46} P_{35} \psi_{12;12,34}^{123,45} \right. \\ & \quad \left. - (P_{45} + P_{35}) \psi_{12;12,34}^{1234} - P_{35} \psi_{12;12,34}^{12,34,56} \right) \end{aligned} \quad (69)$$

$$\begin{aligned} & \psi_{12;12,34}^{12,34,56} - G_0 T^{12,34} P_{35} P_{46} \psi_{12;12,34}^{12,34,56} = G_0 T^{12,34} \left( P_{35} P_{46} \psi_{12;12,34}^{1234} + (1 - P_{34}) \right. \\ & \quad \left. P_{35} P_{46} \left( \psi_{12;12,34}^{125,34} + \psi_{12;12,34}^{345,12} \right) \right) \end{aligned} \quad (70)$$

It remains to establish the expression for the total state  $\Psi$ . We use (1), (5), (42), (52) together with

permutations and obtain

$$\begin{aligned}
\Psi = & [1 - P_{23} - P_{24} - P_{13} - P_{14} + P_{13}P_{24}] \left[ (1 - P_{34})\psi_{12,123}^{1234} + \psi_{12;12,34}^{1234} \right] \\
& - [1 - P_{23} - P_{24} - P_{13} - P_{14} + P_{13}P_{24}] \\
& \times \left[ ((1 - P_{34})(P_{45} + P_{46} + P_{35} + P_{36}) - (P_{35}P_{46} + P_{36}P_{45}))\psi_{12,123}^{1234} \right. \\
& \left. + (P_{45} + P_{46} + P_{35} + P_{36} - P_{35}P_{46})\psi_{12;12,34}^{1234} \right] \\
& - [P_{25} + P_{26} + P_{15} + P_{16} - P_{13}P_{25} - P_{13}P_{26} - P_{14}P_{25} - P_{14}P_{26} - P_{15}P_{26}] \\
& \times \left[ (1 - P_{34})\psi_{12,123}^{1234} + \psi_{12;12,34}^{1234} - ((1 - P_{34})(P_{45} + P_{46} + P_{35} + P_{36}) \right. \\
& \left. - (P_{35}P_{46} + P_{36}P_{45}))\psi_{12,123}^{1234} - (P_{45} + P_{46} + P_{35} + P_{36} - P_{35}P_{46})\psi_{12;12,34}^{1234} \right] \\
& + [1 - P_{23} - P_{24} - P_{13} - P_{14} + P_{13}P_{24}] \left[ (1 - P_{34} - P_{35} - P_{36}) \right. \\
& \times (1 - P_{56} - P_{46})\psi_{12,123}^{123,45} + (1 - P_{45} - P_{46} - P_{35} - P_{36} + P_{35}P_{46}) \\
& \times \left. \left( (1 - P_{56}) \left( \psi_{12,12,34}^{125,34} + \psi_{12;12,34}^{345,12} \right) + \psi_{12;12,34}^{12,34,56} \right) \right] \\
& - [P_{25} + P_{26} + P_{15} + P_{16} - P_{13}P_{25} - P_{13}P_{26} - P_{14}P_{25} - P_{14}P_{26} - P_{15}P_{26}] \\
& \times \left[ (1 - P_{34} - P_{35} - P_{36})(1 - P_{56} - P_{46})\psi_{12,123}^{123,45} \right. \\
& \left. + (1 - P_{45} - P_{46} - P_{35} - P_{36} + P_{35}P_{46}) \right. \\
& \times \left. \left( (1 - P_{56}) \left( \psi_{12,12,34}^{125,34} + \psi_{12;12,34}^{345,12} \right) + \psi_{12;12,34}^{12,34,56} \right) \right] \quad (71)
\end{aligned}$$

The first piece

$$\Psi_4 \equiv [1 - P_{23} - P_{24} - P_{13} - P_{14} + P_{13}P_{24}] \left[ (1 - P_{34})\psi_{12,123}^{1234} + \psi_{12;12,34}^{1234} \right] \quad (72)$$

has exactly the form for a 4-nucleon bound state (12; 14) based on the two Yakubovsky components  $\psi_{12,123}^{1234}$  and  $\psi_{12;12,34}^{1234}$ . Now for 6 nucleons these two amplitudes depend not only on the momenta of nucleons 1 to 4 but also on the momenta of nucleons 5 and 6. In the spirit of the effective 3-body model  $\alpha - n - n\Psi_4$  factorizes into a product of the  $\alpha$ -state and the wave function for the two neutrons. The next two pieces, still related to the same two Yakubovsky components, antisymmetrize the nucleons 5 and 6 in relation to the nucleons 1 to 4. The remaining two pieces, going with the additional three Yakubovsky components  $\psi_{12,123}^{123,45}$ ,  $\psi_{12,12,34}^{125,34} + \psi_{12;12,34}^{345,12}$  and  $\psi_{12;12,34}^{12,34,56}$ , go clearly beyond the effective 3-body model and allow for additional sub clusterings of different types. In addition one has to keep in mind that the most general form (71) allows many more distributions of neutrons and protons in the sub clusters than restricted in the effective  $\alpha - n - n$  picture.

#### 4 Technicalities for a Numerical Implementation

The 5 independent amplitudes require 5 different Jacobi momenta. For  $\psi_{12,34}^{123}$  we choose

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) \\ \mathbf{a}_2 &= \frac{1}{3}(2\mathbf{k}_3 - \mathbf{k}_1 - \mathbf{k}_2) \\ \mathbf{a}_3 &= \frac{1}{4}(3\mathbf{k}_4 - \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \\ \mathbf{a}_4 &= \frac{1}{2}(\mathbf{k}_5 - \mathbf{k}_6) \\ \mathbf{a}_5 &= \frac{1}{3}(2(\mathbf{k}_5 + \mathbf{k}_6) - \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \end{aligned} \quad (73)$$

Then the individual momenta (under the condition  $\sum_i \mathbf{k}_i = 0$ ) in terms of those Jacobi momenta are

$$\begin{aligned} \mathbf{k}_1 &= \mathbf{a}_1 - \frac{1}{2}\mathbf{a}_2 - \frac{1}{3}\mathbf{a}_3 - \frac{1}{4}\mathbf{a}_5 \\ \mathbf{k}_2 &= -\mathbf{a}_1 - \frac{1}{2}\mathbf{a}_2 - \frac{1}{3}\mathbf{a}_3 - \frac{1}{4}\mathbf{a}_5 \\ \mathbf{k}_3 &= \mathbf{a}_2 - \frac{1}{3}\mathbf{a}_3 - \frac{1}{4}\mathbf{a}_5 \\ \mathbf{k}_4 &= \mathbf{a}_3 - \frac{1}{4}\mathbf{a}_5 \\ \mathbf{k}_5 &= \mathbf{a}_4 + \frac{1}{2}\mathbf{a}_5 \end{aligned} \quad (74)$$

The kinetic energy is

$$\sum_{i=1}^6 \frac{k_i^2}{2m} = \frac{1}{m} \left( a_1^2 + \frac{3}{4}a_2^2 + \frac{2}{3}a_3^2 + a_4^2 + \frac{3}{8}a_5^2 \right) \quad (75)$$

The remaining choices of Jacobi momenta are given in Appendix A.

In a partial wave decomposition the basis states suitable for  $\psi_{12,34}^{123}$  are

$$\begin{aligned} |a_1 a_2 a_3 a_4 a_5 \alpha_1\rangle &\equiv |a_1 a_2 a_3 a_4 a_5, (l_1 s_{12}) j_1 \left( l_2 \frac{1}{2} \right) j_2 (j_1 j_2) I_3 \left( l_3 \frac{1}{2} \right) j_4 (I_3 j_4) I_4 (l_5 s_{56}) j_5 \\ &\quad (l_4 j_5) I_5 (I_4 I_5) J M \rangle \left| \left( t_{12} \frac{1}{2} \right) t_3 \left( t_3 \frac{1}{2} \right) t_4 (t_4 t_{56}) T M_T \right\rangle \end{aligned} \quad (76)$$

Here the orbital angular momenta  $l_i$  go with the  $\mathbf{a}_i$ ,  $s_{ij}$  are two-body spins for particles  $ij$ ,  $j_i$  are total 1- and 2-body angular momenta coupled out of orbital and spin angular momenta,  $I_3$  and  $I_4$  are total 3- and 4-body angular momenta,  $I_5$  the total angular momentum of particles 5 and 6 relative to particles 1–4 and finally  $I_4$  and  $I_5$  are coupled to  $J$ , the conserved total 6-body angular momentum. The second state in (76) refers to isospin in an obvious manner.

Using (76) the amplitude  $\psi_{123}^{1234}$  has the representation

$$|\psi_{123}^{1234}\rangle = \sum_{\alpha_1} \int \Pi_{i=1}^5 da_i a_i^2 |a_1 a_2 a_3 a_4 a_5 \alpha_1\rangle \langle a_1 a_2 a_3 a_4 a_5 \alpha_1 | \psi_{123}^{1234}\rangle \quad (77)$$

where the discrete set of quantum numbers  $\alpha_1$  runs over all values for a given  $J$  and  $T$ .

Thereby antisymmetry requires that  $l_1 + s_{12} + t_{12}$  and  $l_4 + s_{56} + t_{56}$  have to be odd.

Analogous basis states for the other 4 amplitudes and related Jacobi momenta should be obvious. One other example is given below.

If one projects the coupled equations (67)–(70) from the left onto the adequate basis states and expands the 5 amplitudes on the right-hand side like in (77) one faces the task to evaluate the various kernels. As an example out of (67) we take

$$\begin{aligned} \langle a_1 a_2 a_3 a_4 a_5 \alpha_1 | \psi_{12,123}^{1234} \rangle &= -G_0 \langle a_1 a_2 a_3 a_4 a_5 \alpha_1 | T^{123} P_{34} \sum_{\alpha'_1} \int \Pi_{i=1}^5 da'_i a_i'^2 |a'_1 a'_2 a'_3 a'_4 a'_5 \alpha'_1\rangle \\ &\times \langle a'_1 a'_2 a'_3 a'_4 a'_5 \alpha'_1 | \psi_{12,123}^{1234} \rangle + G_0 \langle a_1 a_2 a_3 a_4 a_5 \alpha_1 | T^{123} \left| \sum_{\alpha'_2} \int \Pi_{i=1}^5 db'_i b_i'^2 \right| b'_1 b'_2 b'_3 b'_4 b'_5 \alpha'_2 \rangle \\ &\times \langle b'_1 b'_2 b'_3 b'_4 b'_5 \alpha'_2 | \psi_{12,12,34}^{1234} \rangle + \dots \end{aligned} \quad (78)$$

where the  $\dots$  refer to the remaining operators and amplitudes and the b-states are related to  $\psi_{12,12,34}^{1234}$ .

Using techniques like the ones presented in (12; 20; 17; 21) it is straightforward, though tedious, to generate the kernels like  $\langle a_1 a_2 a_3 a_4 a_5 \alpha_1 | T^{123} P_{34} | a'_1 a'_2 a'_3 a'_4 a'_5 \alpha'_1 \rangle$  or  $\langle b_1 b_2 b_3 b_4 b_5 \alpha_2 | T^{12,34} (1 - P_{34}) (P_{45} + P_{46}) | a'_1 a'_2 a'_3 a'_4 a'_5 \alpha'_1 \rangle$ .

In the course of the required recoupling among the different Jacobi momenta the variables for the 5 amplitudes on the right-hand sides are in general linear combinations of intermediate integration variables which include angles besides momentum magnitudes. An example illustrates that situation:

$$H \equiv P_{45} \psi_{12,123}^{1234} \quad (79)$$

We project onto the basis states for Jacobi momenta of type b given in Appendix A:

$$\begin{aligned} |b\rangle &\equiv |b_1 b_2 b_3 b_4 b_5; (l_1 s_{12}) j_1 (l_2 s_{34}) j_2 (j_1 j_2) S(LS) I(l_4 s_{56}) j_5 (l_5 j_5) I_5 (II_5) JM\rangle \\ &\times |(t_{12} t_{34}) t_{1-4} (t_{1-4} t_{56}) T M_T\rangle \end{aligned} \quad (80)$$

where the orbital angular momenta  $l_i, i \neq 3$  go with  $\mathbf{b}_i$  and  $L$  goes with  $\mathbf{b}_3$ . The 2-body spins are  $s_{12}, s_{34}$  and  $s_{56}$ ,  $I$  is the total angular momentum for particles 1–4 and  $I_5$  the total angular momentum of the pair 56 against the subsystem 1–4. They are coupled to the total angular momentum  $J$ , which is conserved. The isospin coupling should be obvious.

For the sake of simplicity we choose s-waves which simplifies (80) to

$$\begin{aligned} |b\rangle &\equiv \delta_{SI} \delta_{s_{12} j_1} \delta_{s_{34} j_2} \delta_{j_5 I_5} \delta_{s_{56} j_5} \\ &\times |b_1 b_2 b_3 b_4 b_5; (s_{12} s_{34}) S(S s_{56}) JM\rangle |(t_{12} t_{34}) t_{1-4} (t_{1-4} t_{56}) T M_T\rangle \end{aligned} \quad (81)$$

The basis states (76) related to the Jacobi momenta of type a and restricted to s-waves are

$$|a\rangle = \delta_{s_{12}j_1} \delta_{j_2 \frac{1}{2}} \delta_{j_4 \frac{1}{2}} \delta_{j_5 s_{56}} \delta_{j_5 I_5} |a_1 a_2 a_3 a_4 a_5\rangle \\ \times \left| \left( s_{12} \frac{1}{2} \right) I_3 \left( I_3 \frac{1}{2} \right) I_4 (I_4 s_{56}) JM \right\rangle \left| \left( t_{12} \frac{1}{2} \right) t_3 \left( t_3 \frac{1}{2} \right) t_4 (t_4 t_{56}) T M_T \right\rangle \quad (82)$$

Then  $\psi_{12,123}^{1234}$  has the representation

$$|\psi_{12,123}^{1234}\rangle \equiv \sum_{\alpha_1} \delta \cdots \int \Pi_{i=1}^5 da_i a_i^2 |a_1 a_2 a_3 a_4 a_5\rangle |spin\rangle_a |isospin\rangle_a \langle a | \psi_{12,123}^{1234} \rangle \quad (83)$$

and H projected from the left is

$$\langle b | H \rangle = \delta_{SI} \delta_{s_{12}j_1} \delta_{s_{34}j_2} \delta_{j_5 I_5} \delta_{s_{56}j_5} \\ \times \left\langle \left( t_{12} t_{34} \right) t_{1-4} \left( t_{1-4} t_{56} \right) T M_T \right| \left\langle \left( s_{12} s_{34} \right) S (S s_{56}) J M \right| \langle b_1 b_2 b_3 b_4 b_5 | P_{45} \\ \times \sum_{\alpha'_1} \delta \cdots \int \Pi_{i=1}^5 da_i a_i^2 |a_1 a_2 a_3 a_4 a_5\rangle \left| \left( s'_{12} \frac{1}{2} \right) I'_3 \left( I'_3 \frac{1}{2} \right) I'_4 (I'_4 s'_{56}) J M \right\rangle \\ \times \left| \left( t'_{12} \frac{1}{2} \right) t'_3 \left( t'_3 \frac{1}{2} \right) t'_4 (t'_4 t'_{56}) T M_T \right\rangle \langle a | \psi_{12,123}^{1234} \rangle \quad (84) \\ \equiv \delta \cdots \sum_{\alpha_1} \delta \cdots \int \Pi_{i=1}^5 da_i a_i^2 \langle isospin | P_{45}^{isospin} | isospin \rangle_a \\ \times_b \langle spin | P_{45}^{spin} | spin \rangle_a \langle b_1 b_2 b_3 b_4 b_5 | P_{45}^{mom} | a_1 a_2 a_3 a_4 a_5 \rangle \langle a | \psi_{12,123}^{1234} \rangle$$

The permutation is separated into the 3 spaces: isospin, spin, and momentum, and the  $\delta' s \cdots$  are the strings of Kronecker symbols.

The isospin- and spin-matrix elements can be calculated in a standard manner:

$${}_b \langle isospin | P_{45}^{isospin} | isospin \rangle_a = \delta_{TT'} \delta_{M_T m_T'} \delta_{t_{12} t_{12}'} (-)^{t_{12}+t_{1-4}+1} \sqrt{\hat{t}_3' \hat{t}_{34} \hat{t}_{1-4} \hat{t}_{56} \hat{t}_4' \hat{t}_{56}'} \left\{ \begin{matrix} t_{12} & \frac{1}{2} & t_3' \\ \frac{1}{2} & t_{1-4} & t_{34} \end{matrix} \right\} \left\{ \begin{matrix} t_3' & \frac{1}{2} & t_{1-4} \\ \frac{1}{2} & \frac{1}{2} & t_{56} \\ t_4' & t_{56}' & T \end{matrix} \right\} \quad (85)$$

$${}_b \langle spin | P_{45}^{spin} | spin \rangle_a = \delta_{s_{12} s_{12}'} (-)^{s_{12}+S+1} \sqrt{\hat{I}_3' \hat{s}_{34} \hat{S} \hat{s}_{56} \hat{I}_4' \hat{s}_{56}'} \left\{ \begin{matrix} s_{12} & \frac{1}{2} & I_3' \\ \frac{1}{2} & S & s_{34} \end{matrix} \right\} \left\{ \begin{matrix} I_3' & \frac{1}{2} & S \\ \frac{1}{2} & \frac{1}{2} & s_{56} \\ I_4' & s_{56}' & J \end{matrix} \right\} \quad (86)$$

For the momentum space part we insert a complete basis and obtain

$$\begin{aligned} \langle b_1 b_2 b_3 b_4 b_5 | P_{45}^{mom} = \int d^3 b_1' \cdots d^3 b_5' \langle b_1 b_2 b_3 b_4 b_5 | \mathbf{b}_1' \mathbf{b}_2' \mathbf{b}_3' \mathbf{b}_4' \mathbf{b}_5' \rangle \langle \mathbf{b}_1' \mathbf{b}_2' \mathbf{b}_3' \mathbf{b}_4' \mathbf{b}_5' | P_{45}^{mom} \\ = \left( \frac{1}{\sqrt{4\pi}} \right)^5 \int d\hat{b}_1' \cdots d\hat{b}_5' \langle b_1 \hat{b}_1' b_2 \hat{b}_2' b_3 \hat{b}_3' b_4 \hat{b}_4' b_5 \hat{b}_5' | P_{45}^{mom} \end{aligned} \quad (87)$$

The transposition  $P_{45}^{mom}$  acting to the left leads to a state with the same quantum numbers but different meaning. Particles 4 and 5 are interchanged. That state can be reexpressed again in terms of the old b-state using the relation between the Jacobi momenta  $\mathbf{b}_1, \dots, \mathbf{b}_5$  and the Jacobi momenta with particles 4 and 5 interchanged. It results

$$\begin{aligned} \langle \mathbf{b}_1 \mathbf{b}_2 \mathbf{b}_3 \mathbf{b}_4 \mathbf{b}_5 | P_{45} = \left\langle \mathbf{b}_1, \frac{1}{2} \left( \mathbf{b}_2 - \frac{1}{2} \mathbf{b}_3 - \mathbf{b}_4 - \frac{3}{4} \mathbf{b}_5 \right), \frac{1}{2} \left( -\mathbf{b}_2 + \frac{3}{2} \mathbf{b}_3 - \mathbf{b}_4 - \frac{3}{4} \mathbf{b}_5 \right), \right. \\ \left. \frac{1}{2} \left( -\mathbf{b}_2 - \frac{1}{2} \mathbf{b}_3 + \mathbf{b}_4 - \frac{3}{4} \mathbf{b}_5 \right), - \left( \mathbf{b}_2 + \frac{1}{2} \mathbf{b}_3 + \mathbf{b}_4 - \frac{1}{4} \mathbf{b}_5 \right) \right| \quad (88) \end{aligned}$$

Consequently

$$\begin{aligned} \langle b_1 b_2 b_3 b_4 b_5 | P_{45}^{mom} = \left( \frac{1}{\sqrt{4\pi}} \right)^5 \int d\hat{b}_1' \cdots d\hat{b}_5' \\ \left\langle b_1 \hat{b}_1', \frac{1}{2} \left( b_2 \hat{b}_2' - \frac{1}{2} b_3 \hat{b}_3' - b_4 \hat{b}_4' - \frac{3}{4} b_5 \hat{b}_5' \right), \frac{1}{2} \left( -b_2 \hat{b}_2' + \frac{3}{2} b_3 \hat{b}_3' - b_4 \hat{b}_4' - \frac{3}{4} b_5 \hat{b}_5' \right), \right. \\ \left. \frac{1}{2} \left( -b_2 \hat{b}_2' - \frac{1}{2} b_3 \hat{b}_3' + b_4 \hat{b}_4' - \frac{3}{4} b_5 \hat{b}_5' \right), - \left( b_2 \hat{b}_2' + \frac{1}{2} b_3 \hat{b}_3' + b_4 \hat{b}_4' - \frac{1}{4} b_5 \hat{b}_5' \right) \right| \quad (89) \end{aligned}$$

The state  $|\mathbf{b}_1 \cdots \mathbf{b}_5\rangle$  can be reexpressed in terms of the state  $|\mathbf{a}_1 \cdots \mathbf{a}_5\rangle$  as

$$|\mathbf{b}_1 \mathbf{b}_2 \mathbf{b}_3 \mathbf{b}_4 \mathbf{b}_5\rangle = |\mathbf{b}_1, \frac{2}{3}(\mathbf{b}_2 - \mathbf{b}_3), -\frac{1}{2}(2\mathbf{b}_2 + \mathbf{b}_3), \mathbf{b}_4, \mathbf{b}_5\rangle \quad (90)$$

Consequently using (89) and (90) one obtains

$$\begin{aligned}
& \langle b_1 b_2 b_3 b_4 b_5 | P_{45}^{mom} \int \Pi_{i=1}^5 da_i a_i^2 | a_1 a_2 a_3 a_4 a_5 \rangle \langle a_1 a_2 a_3 a_4 a_5 | \psi_{12,123}^{1234} \rangle \\
&= \int d\hat{b}'_1 \cdots d\hat{b}'_5 \left\langle b_1, \frac{1}{3} \left| 2b_2 \hat{b}'_2 - 2b_3 \hat{b}'_3 \right|, \frac{1}{2} \left| \frac{1}{2} b_2 \hat{b}'_2 + \frac{1}{4} b_3 \hat{b}'_3 - \frac{3}{4} b_4 \hat{b}'_4 - \frac{9}{8} b_5 \hat{b}'_5 \right|, \right. \\
&\quad \left. \frac{1}{2} \left| -\frac{1}{2} b_2 \hat{b}'_2 - \frac{1}{2} b_3 \hat{b}'_3 + b_4 \hat{b}'_4 - \frac{3}{4} b_5 \hat{b}'_5 \right|, \right. \\
&\quad \left. \left| b - 2\hat{b}'_2 + \frac{1}{2} b_3 \hat{b}'_3 + b_4 \hat{b}'_4 - \frac{1}{4} b_5 \hat{b}'_5 \right| \right| \psi_{12,123}^{1234} \rangle \left( \frac{1}{\sqrt{4\pi}} \right)^5 \quad (91)
\end{aligned}$$

The angular integration over  $\hat{b}'_1$  yields directly  $4\pi$ . Further one can put  $\hat{b}'_2$  into the z-direction and  $\hat{b}'_3$  into the x-z plane. Therefore

$$\begin{aligned}
& \langle b_1 b_2 b_3 b_4 b_5 | P_{45}^{mom} \int \Pi_{i=1}^5 da_i a_i^2 | a_1 a_2 a_3 a_4 a_5 \rangle \langle a_1 a_2 a_3 a_4 a_5 | \psi_{12,123}^{1234} \rangle \\
&= \sqrt{\pi} \int d\cos\theta'_3 d\hat{b}'_4 d\hat{b}'_5 \left\langle b_1, \frac{1}{3} \left| 2b_2 \hat{b}'_2 - 2b_3 \hat{b}'_3 \right|, \frac{1}{2} \left| \frac{1}{2} b_2 \hat{b}'_2 + \frac{1}{4} b_3 \hat{b}'_3 - \frac{3}{4} b_4 \hat{b}'_4 - \frac{9}{8} b_5 \hat{b}'_5 \right|, \right. \\
&\quad \left. \frac{1}{2} \left| -\frac{1}{2} b_2 \hat{b}'_2 - \frac{1}{2} b_3 \hat{b}'_3 + b_4 \hat{b}'_4 - \frac{3}{4} b_5 \hat{b}'_5 \right|, \left| b_2 \hat{b}'_2 + \frac{1}{2} b_3 \hat{b}'_3 + b_4 \hat{b}'_4 - \frac{1}{4} b_5 \hat{b}'_5 \right| \right| \psi_{12,123}^{1234} \rangle \quad (92)
\end{aligned}$$

This is an example where a 4-dimensional interpolation appears necessary. Therefore if the momentum magnitudes are discretized choosing for each one a certain grid, interpolations are inevitable.

In the 3- and 4-nucleon problems cubic Hermitean spline interpolation turned out to be very efficient (22). Thus a 5-dimensional interpolation, for instance, has the form

$$f_{ijklm}(a_1 a_2 a_3 a_4 a_5) = \sum_{r=0}^3 \sum_{s=0}^3 \sum_{t=0}^3 \sum_{u=0}^3 \sum_{v=0}^3 S_r(a_1) S_s(a_2) S_t(a_3) S_u(a_4) S_v(a_5) f(a_{1r} a_{2s} a_{3t} a_{4u} a_{5v}) \quad (93)$$

where  $ijklm$  denotes the 5-dimensional cubus around the point  $a_1 a_2 a_3 a_4 a_5$  and  $a_{ik}$  denotes the grid points for the variable  $a_i$ .

For  $a_1$ , for instance, the 4 grid points related to  $a_i$  are  $a_{10} < a_{11} \leq a_1 \leq a_{12} < a_{13}$  and similar for the other variables. Here for the sake of a simpler notation we renumbered the grid points in that context.

Further  $f$  is the function to be interpolated and  $f_{ijklm}$  the interpolating one. The spline functions are given in Appendix B and the conditions underlying that form (93) can be found in (22).

The coupled set (67)–(70) in a matrix notation has the schematic structure

$$\eta(E) \psi = K(E) \psi \quad (94)$$

where  $E$  is the searched for energy eigenvalue at which the auxiliary kernel eigenvalue  $\eta(E) = 1$ . For 3- and 4-nucleon bound states a Lanczos type algorithm turned out to be very efficient (17; 23). Starting from an arbitrary initial  $\psi = \psi_0$  one generates by consecutive applications of  $K$  a sequence of amplitudes  $\psi_n$ , which after orthogonalisation form a basis into which  $\psi$  is expanded. It turn out that a reasonably small



number of K-applications (of the order of 10–20) is sufficient, which leads to an algebraic eigenvalue problem of rather low dimension. Then the energy is varied such that one reaches  $\eta(E) = 1$ .

If one regards the sub clustering underlying the 5 amplitudes only two of them,  $\psi_{12,123}^{1234}$  and  $\psi_{12,12,34}^{1234}$ , are related to the very approximative effective 3-body model of an inert  $\alpha$ -core and two neutrons. The total isospin quantum numbers of the  ${}^6\text{He}$  ground state are  $T = 1$  and  $M_T = -1$  (if we define the magnetic isospin quantum number of the neutron as  $-\frac{1}{2}$ ).

Now even these two amplitudes depending on the Jacobi momenta of type a and b, (73) and (95), respectively, are not restricted to  $t_4 = 0$  and  $t_{56} = 1$  in case of  $\psi_{12,123}^{1234}$  but also allow  $t_4 = 1$  and  $t_{56} = 1$ ,  $t_4 = 2$  and  $t_{56} = 1$  and  $t_4 = 1$  and  $t_{56} = 0$ . Similarly the “deuteron-deuteron” like substructures of  $\psi_{12,12,34}^{1234}$  are not restricted to  $t_{12} = t_{34} = 0$  and  $t_{56} = 1$  but also other two-body isospins are allowed which do not built up a  $t = 0\alpha$ -core. The amplitudes  $\psi_{12,123}^{123,45}$  going with Jacobi momenta of type c, (98), refer to a 3-body together with a two-body sub clustering, which is also not present in the effective 3-body model. The linear combinations  $\psi_{12,12,34}^{125,34} + \psi_{12,12,34}^{345,12}$  refer again to a 3-body together with a 2-body sub clustering, where the underlying fragmentation related to 2-body fragments differs from  $\psi_{12,123}^{123,45}$ . And again this is beyond the effective 3-body model. Finally  $\psi_{12,12,34}^{12,34,56}$  allows for several additional 2-body sub clusters which are not contained in the effective 3-body model, either.

If one would add another step in the Yakubovsky scheme, namely to 2-body fragmentations  $a_2$ , the resulting amplitudes  $\psi_{a_5,a_4,a_3}^{a_2}$  would point to 5-body subclusters together with a single nucleon or to two 3-body subclusters (like  ${}^3\text{H}-{}^3\text{H}$ ) in addition to 4-body and 2-body subclusters. Now all those additional structures are of course also generated by the coupled system (67)–(70) ending with  $a_3$  fragmentation, which we presented. In other words that Yakubovsky scheme is complete and delivers an exact description of the 6-nucleon problem.

## 5 Summary

The Yakubovsky equations have been derived long time ago by Yakubovsky (19). Therefore the application presented here could have been given also long time ago. It is, however, only now after the experiences with 3- and 4-nucleon problems in the Faddeev–Yakubovsky schemes that the technical expertise has been developed in the last decades and the very strong increase of computer power just recently achieved allows to attack the 6-body problem in that exact formulation. Therefore we felt it is timely to work out that scheme for that system. Another argument is the development of nuclear forces in a systematic manner in the realm of effective field theory and based on chiral symmetry. Two-, three-, and four-nucleon forces have been derived consistently to each other and they are waiting to be applied in light nuclear systems and checked against nature. Several tests in that spirit already appeared (3; 4; 5; 6; 17; 24; 25) but for the purpose of benchmarking the exact approach in the Yakubovsky scheme is strongly recommended.

Here we restricted the formulation to two-nucleon forces only but the inclusion of three-nucleon forces can easily be done like pioneered in (13).

In Sect. 2 we used the general basic and standard formulation, where  $a_n$  points to  $n$ -body fragmentations for a system of  $N > n$  particles.

We worked out that scheme ending with  $a_3$  in the spirit of the usually applied though approximate effective  $\alpha - n - n$  3-body model.

Though the step to  $a_2$  could be easily done, ending with  $a_3$  still includes exactly the whole dynamics.

The Pauli principle is then exactly incorporated in Sect. 3 leading to a set of 5 coupled equations for 5 independent Yakubovsky components, which built up the total state.

The technical performance in a partial wave decomposition is only touched in Sect. 4. The 5 different Jacobi momenta as well as a necessary multi-dimensional interpolation scheme, like modified cubic Hermitean splines, are given. For solving the high dimensional energy eigenvalue problem of the 5 coupled equations we point to the Lanczos type algorithm, which turned out to be very efficient in the 3- and 4-nucleon problem. It remains to work out the partial wave projected kernels, which is straightforward and can be carried through along the lines cited above. An example for that is presented.

We expect that on the most modern supercomputers with parallel architecture this formulation can be numerically mastered. Then the step to six-nucleon scattering like  $d - \alpha$  or quite interesting the continuum  $nn - \alpha$  revealing the resonances in  ${}^6\text{He}$  appears also to be feasible. Recently it was shown (26) that the moving logarithmic singularities in three-nucleon scattering, which in the past was a stumbling block, though meanwhile very well under control, can nowadays be totally avoided leading to a very simple pole structure in the Faddeev kernel. The corresponding trick can also be applied to the 4N Yakubovsky kernel in the continuum (A. Nogga, Private communication) and it remains to be seen whether this is also true beyond  $A = 4$ . In such a case continuum calculations are hardly more difficult than bound state calculations.

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## A Jacobi Momenta Related to the Independent Yakubovsky Components

Here we display various Jacobi momenta related to the independent Yakubovsky components.

To  $\psi_{12,12,34}^{1234}$  belongs

$$\begin{aligned}
 \mathbf{b}_1 &= \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) = \mathbf{a}_1 \\
 \mathbf{b}_2 &= \frac{1}{2}(\mathbf{k}_3 - \mathbf{k}_4) \\
 \mathbf{b}_3 &= \frac{1}{2}(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \\
 \mathbf{b}_4 &= \frac{1}{2}(\mathbf{k}_5 - \mathbf{k}_6) = \mathbf{a}_4 \\
 \mathbf{b}_5 &= \frac{1}{3}(2(\mathbf{k}_5 + \mathbf{k}_6) - \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) = \mathbf{a}_5
 \end{aligned} \tag{95}$$

The individual momenta are expressed in terms of those Jacobi momenta:

$$\begin{aligned}
 \mathbf{k}_1 &= \mathbf{b}_1 + \frac{1}{2}\mathbf{b}_3 - \frac{1}{4}\mathbf{b}_5 \\
 \mathbf{k}_2 &= -\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_3 - \frac{1}{4}\mathbf{b}_5 \\
 \mathbf{k}_3 &= \mathbf{b}_2 - \frac{1}{2}\mathbf{b}_3 - \frac{1}{4}\mathbf{b}_5 \\
 \mathbf{k}_4 &= -\mathbf{b}_2 - \frac{1}{2}\mathbf{b}_3 - \frac{1}{4}\mathbf{b}_5 \\
 \mathbf{k}_5 &= \mathbf{b}_4 + \frac{1}{2}\mathbf{b}_5
 \end{aligned} \tag{96}$$

The kinetic energy is

$$\sum_{i=1}^6 \frac{k_i^2}{2m} = \frac{1}{2m} \left( 2b_1^2 + 2b_2^2 + b_3^2 + 2b_4^2 + \frac{3}{4}b_5^2 \right) \tag{97}$$

To  $\psi_{12,123}^{123,45}$  belongs

$$\begin{aligned}
 \mathbf{c}_1 &= \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) = \mathbf{a}_1 \\
 \mathbf{c}_2 &= \frac{1}{3}(2\mathbf{k}_3 - \mathbf{k}_1 - \mathbf{k}_2) = \mathbf{a}_2 \\
 \mathbf{c}_3 &= \frac{1}{2}(\mathbf{k}_4 - \mathbf{k}_5) \\
 \mathbf{c}_4 &= \frac{1}{3}(\mathbf{k}_4 + \mathbf{k}_5 - 2\mathbf{k}_6) \\
 \mathbf{c}_5 &= \frac{1}{2}(\mathbf{k}_4 + \mathbf{k}_5 + \mathbf{k}_6 - \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3)
 \end{aligned} \tag{98}$$

or

$$\begin{aligned}
\mathbf{k}_1 &= \mathbf{c}_1 - \frac{1}{2}\mathbf{c}_2 - \frac{1}{3}\mathbf{c}_5 \\
\mathbf{k}_2 &= -\mathbf{c}_1 - \frac{1}{2}\mathbf{c}_2 - \frac{1}{3}\mathbf{c}_5 \\
\mathbf{k}_3 &= \mathbf{c}_2 - \frac{1}{3}\mathbf{c}_5 \\
\mathbf{k}_4 &= \mathbf{c}_3 + \frac{1}{2}\mathbf{c}_4 + \frac{1}{3}\mathbf{c}_5 \\
\mathbf{k}_5 &= -\mathbf{c}_3 + \frac{1}{2}\mathbf{c}_4 + \frac{1}{3}\mathbf{c}_5 \\
\mathbf{k}_6 &= -\mathbf{c}_4 + \frac{1}{3}\mathbf{c}_5
\end{aligned} \tag{99}$$

and the kinetic energy is

$$\sum_{i=1}^6 \frac{k_i^2}{2m} = \frac{1}{m}c_1^2 + \frac{3}{4m}c_2^2 + \frac{1}{m}c_3^2 + \frac{3}{4m}c_4^2 + \frac{1}{3m}c_5^2 \tag{100}$$

To  $\psi_{12;12,34}^{125,34}$  belongs

$$\begin{aligned}
\mathbf{d}_1 &= \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) = \mathbf{a}_1 \\
\mathbf{d}_2 &= \frac{1}{3}(2\mathbf{k}_5 - \mathbf{k}_1 - \mathbf{k}_2) \\
\mathbf{d}_3 &= \frac{1}{2}(\mathbf{k}_3 - \mathbf{k}_4) = \mathbf{b}_2 \\
\mathbf{d}_4 &= \frac{1}{3}(\mathbf{k}_3 + \mathbf{k}_4 - 2\mathbf{k}_6) \\
\mathbf{d}_5 &= \frac{1}{3}(\mathbf{k}_3 + \mathbf{k}_4 + \mathbf{k}_6 - \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_5)
\end{aligned} \tag{101}$$

or

$$\begin{aligned}
\mathbf{k}_1 &= \mathbf{d}_1 - \frac{1}{2}\mathbf{d}_2 - \frac{1}{3}\mathbf{d}_5 \\
\mathbf{k}_2 &= -\mathbf{d}_1 - \frac{1}{2}\mathbf{d}_2 - \frac{1}{3}\mathbf{d}_5 \\
\mathbf{k}_3 &= \mathbf{d}_3 + \frac{1}{2}\mathbf{d}_4 + \frac{1}{3}\mathbf{d}_5 \\
\mathbf{k}_4 &= -\mathbf{d}_3 + \frac{1}{2}\mathbf{d}_4 + \frac{1}{3}\mathbf{d}_5 \\
\mathbf{k}_5 &= \mathbf{d}_2 - \frac{1}{3}\mathbf{d}_5 \\
\mathbf{k}_6 &= -\mathbf{d}_4 + \frac{1}{3}\mathbf{d}_5
\end{aligned} \tag{102}$$

and the kinetic energy is

$$\sum_{i=1}^6 \frac{k_i^2}{2m} = \frac{1}{m}d_1^2 + \frac{3}{4m}d_2^2 + \frac{1}{m}d_3^2 + \frac{3}{4m}d_4^2 + \frac{1}{3m}d_5^2 \tag{103}$$

To  $\psi_{12;12,34}^{345,12}$  belongs

$$\begin{aligned}
 \mathbf{e}_1 &= \frac{1}{2}(\mathbf{k}_3 - \mathbf{k}_4) = \mathbf{b}_2 \\
 \mathbf{e}_2 &= \frac{1}{3}(2\mathbf{k}_5 - \mathbf{k}_3 - \mathbf{k}_4) \\
 \mathbf{e}_3 &= \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) = \mathbf{a}_1 \\
 \mathbf{e}_4 &= \frac{1}{3}(\mathbf{k}_1 + \mathbf{k}_2 - 2\mathbf{k}_6) \\
 \mathbf{e}_5 &= \frac{1}{3}(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_6 - \mathbf{k}_3 - \mathbf{k}_4 - \mathbf{k}_5)
 \end{aligned} \tag{104}$$

or

$$\begin{aligned}
 \mathbf{k}_1 &= \mathbf{e}_3 + \frac{1}{2}\mathbf{e}_4 + \frac{1}{3}\mathbf{e}_5 \\
 \mathbf{k}_2 &= -\mathbf{e}_3 + \frac{1}{2}\mathbf{e}_4 + \frac{1}{3}\mathbf{e}_5 \\
 \mathbf{k}_3 &= \mathbf{e}_1 - \frac{1}{2}\mathbf{e}_2 - \frac{1}{3}\mathbf{e}_5 \\
 \mathbf{k}_4 &= -\mathbf{e}_1 - \frac{1}{2}\mathbf{e}_2 - \frac{1}{3}\mathbf{e}_5 \\
 \mathbf{k}_5 &= \mathbf{e}_2 - \frac{1}{3}\mathbf{e}_5 \\
 \mathbf{k}_6 &= -\mathbf{e}_4 + \frac{1}{3}\mathbf{e}_5
 \end{aligned} \tag{105}$$

and the kinetic energy is

$$\sum_{i=1}^6 \frac{k_i^2}{2m} = \frac{1}{m}e_1^2 + \frac{3}{4m}e_2^2 + \frac{1}{m}e_3^2 + \frac{3}{4m}e_4^2 + \frac{1}{3m}e_5^2 \tag{106}$$

To  $\psi_{12;12,34}^{12,34,56}$  belongs

$$\begin{aligned}
 \mathbf{f}_1 &= \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) = \mathbf{a}_1 \\
 \mathbf{f}_2 &= \frac{1}{2}(\mathbf{k}_3 - \mathbf{k}_4) = \mathbf{b}_2 \\
 \mathbf{f}_3 &= \frac{1}{2}(\mathbf{k}_5 - \mathbf{k}_6) = \mathbf{a}_4 \\
 \mathbf{f}_4 &= \frac{1}{2}(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \\
 \mathbf{f}_5 &= \frac{1}{3}(2(\mathbf{k}_5 + \mathbf{k}_6) - \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) = \mathbf{b}_5
 \end{aligned} \tag{107}$$

or

$$\begin{aligned}
\mathbf{k}_1 &= \mathbf{f}_1 + \frac{1}{2}\mathbf{f}_4 - \frac{1}{4}\mathbf{f}_5 \\
\mathbf{k}_2 &= -\mathbf{f}_1 + \frac{1}{2}\mathbf{f}_4 - \frac{1}{4}\mathbf{f}_5 \\
\mathbf{k}_3 &= \mathbf{f}_2 - \frac{1}{2}\mathbf{f}_4 - \frac{1}{4}\mathbf{f}_5 \\
\mathbf{k}_4 &= -\mathbf{f}_2 - \frac{1}{2}\mathbf{f}_4 - \frac{1}{4}\mathbf{f}_5 \\
\mathbf{k}_5 &= \mathbf{f}_3 + \frac{1}{2}\mathbf{f}_5 \\
\mathbf{k}_6 &= -\mathbf{f}_3 + \frac{1}{2}\mathbf{f}_5
\end{aligned} \tag{108}$$

and the kinetic energy is

$$\sum_{i=1}^6 \frac{k_i^2}{2m} = \frac{1}{m}f_1^2 + \frac{1}{m}f_2^2 + \frac{1}{m}f_3^2 + \frac{1}{4m}f_4^2 + \frac{3}{8m}f_5^2 \tag{109}$$

## B Modified Spline Functions

Choosing four grid points  $x_0, x_1, x_2$ , and  $x_3$  such that  $x_1 \leq x \leq x_2$  the modified spline functions (22) are

$$\begin{aligned}
S_0(x) &= -\phi_3(x) \frac{x_2 - x_1}{x_1 - x_0} \frac{1}{x_2 - x_0} \\
S_1(x) &= \phi_1(x) + \phi_3(x) \left( \frac{x_2 - x_1}{x_1 - x_0} - \frac{x_1 - x_0}{x_2 - x_1} \right) \frac{1}{x_2 - x_0} - \phi_4(x) \frac{x_3 - x_2}{x_2 - x_1} \frac{1}{x_3 - x_1} \\
S_2(x) &= \phi_2(x) + \phi_3(x) \frac{x_1 - x_0}{x_2 - x_1} \frac{1}{x_2 - x_0} + \phi_4(x) \left( \frac{x_3 - x_2}{x_2 - x_1} - \frac{x_2 - x_1}{x_3 - x_2} \right) \frac{1}{x_3 - x_1} \\
S_3(x) &= \phi_4(x) \frac{x_2 - x_1}{x_3 - x_2} \frac{1}{x_3 - x_1}
\end{aligned} \tag{110}$$

with

$$\begin{aligned}
\phi_1(x) &= \frac{(x_2 - x)^2}{(x_2 - x_1)^3} ((x_2 - x_1) + 2(x - x_1)) \\
\phi_2(x) &= \frac{(x_1 - x)^2}{(x_2 - x_1)^3} ((x_2 - x_1) + 2(x_2 - x)) \\
\phi_3(x) &= \frac{(x - x_1)(x - x_2)^2}{(x_2 - x_1)^2} \\
\phi_4(x) &= \frac{(x - x_1)^2(x - x_2)}{(x_2 - x_1)^2}
\end{aligned} \tag{111}$$

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