Chapter 7

Four-body bound states

In the preceding chapters N-body scattering was described theoretically and the two- and three-body bound-state and scattering problems were solved numerically. In this chapter, the next challenge, the four-body problem, is taken on. From a conceptual point of view, the four-body problem is not very much harder than the three-body problem. From a practical point of view, however, it is. The problems which must be dealt with are (i) how to make a correct and efficient numerical implementation of the Faddeev–Yakubovsky equations, and (ii) how to fit this numerical implementation in present-day computers.

These problems were tackled with considerable success by Schut [1991]. He implemented the spline method for the four-body problem, partially exploiting factorizability, following the ideas presented in Chapter 5. Accurate results for s-wave potentials were obtained using a small desktop work station [Schellingerhout et al., 1992]. In this chapter, I report on the method used by Schut, present some new results obtained with his program, and hint at possible improvements.¹

7.1 The four-body Faddeev–Yakubovsky equations

Using Eq. (4.159), we can immediately write down the four-body configuration-space Faddeev–Yakubovsky equations:

\[
(E - H_{a_3}) | \psi^{a_2 a_3} \rangle - V_{a_3} \sum_{\{b_3 \neq a_3\} \subset a_2} | \psi^{a_2 b_3} \rangle = V_{a_3} \sum_{\{b_3 \neq a_3\} \subset a_2} | \psi^{b_3 b_3} \rangle,
\]

or, equivalently:

\[
(E - H_{a_3}) | \psi^{a_2 a_3} \rangle = V_{a_3} \sum_{\{b_3 \neq a_3\} \subset a_2} | \psi^{b_3 b_3} \rangle.
\]

¹The work presented here was for the most part done by Schut as his Master’s degree research project [Schut, 1991]. My contribution consisted of supplying the theoretical insight in the configuration-space Faddeev–Yakubovsky equations and part of the practical formulas. Schut has graciously allowed me to include his implementation and results in this thesis.
These equations can be reduced to the four-body Faddeev equations by summing over \(a_2 \supseteq a_3\) and using Eqs. (4.79) and (4.89):

\[
(E - H_{a_3})\psi^{a_3} = V_{a_3} \sum_{b_3 \neq a_3} |\psi^{b_3}\rangle. \tag{7.3}
\]

The Faddeev amplitudes can equivalently be written as

\[
(E - H_0)|\psi^{a_3}\rangle = V_{a_3} \sum_{b_3} |\psi^{b_3}\rangle. \tag{7.4}
\]

The four-body Faddeev equations can be further reduced to the Schrödinger equation by summing over \(a_3\):

\[
(E - H)|\Psi\rangle = 0. \tag{7.5}
\]

The next step is to choose a specific coordinate representation, and to write the equations in detail. As we have seen in the three-body problem, the different amplitudes are most easily expressed in their own "natural" set of coordinates. Since the Yakubovsky equations couple different amplitudes, it will be necessary to determine the relations between the different coordinate systems. The coupling structure can be summarized as follows: (a) the chain \((ijk)l, (ij)kl\) (where \(i, j, k,\) and \(l\) are particle labels) couples to the chains \((ki)jl, (ki)jl, (ki)jl, (ik)(jl), (ik)jl, (ijk)l, (jk)ij, (jk)il, and (jk)il,\) and \((jk)il, (jk)il,\) and (b) the chain \((ij)(kl), (ij)kl\) couples to \((kl)(ij), (kl)ij, (ikl)j, (kl)ij,\) and \((jkl)i, (kl)ij.\) The corresponding coordinate transformations will be the subject of the next section.

### 7.2 Coordinates in the four-body system

As discussed in Chapter 4, there are eighteen different natural coordinate systems, each associated with a definite partition chain. They can be divided into two groups: (i) the \(3 + 1\) chains (\(i.e.,\) a chain in which the first step is a subdivision of the four-body system into a three-body system and a single body), and (ii) the \(2 + 2\) chains (\(i.e.,\) the first step is a subdivision into two two-body systems). Representatives from both groups are shown in Fig. 4.1. The coordinates are defined by Eq. (4.3). For the sake of simplicity and standardization, I will use the following short-hand notation:

\[
x_{(ijk)l, (ij)kl} = r_i^j, \tag{7.6a}
\]
\[
y_{(ijk)l, (ij)kl} = r_j^k, \tag{7.6b}
\]
\[
z_{(ijk)l, (ij)kl} = r_{ijk}^l, \tag{7.6c}
\]
\[
x_{(ij)(kl), (ij)kl} = r_i^j, \tag{7.6d}
\]
\[
y_{(ij)(kl), (ij)kl} = r_k^l, \tag{7.6e}
\]
\[
z_{(ij)(kl), (ij)kl} = r_{ij}^l. \tag{7.6f}
\]
Note that there is an arbitrariness regarding the signs of $x$ and $y_{(ij)(kl),(ij)kl}$. To cope with this problem, the ordering of the particle labels in the chains will from now on be regarded as relevant. The explicit description of a chain can be replaced by a name (e.g., $a$, $b$, $\ldots$), so that the coordinate systems can be summarized as \{x_a, y_a, z_a\}, or even \{x, y, z\}_a, where $a$ stands for any of the eighteen possible partition chains.

As mentioned in Chapter 4, the eighteen coordinate systems are related to each other by transformations which can be written as products of simple rotations, described by Eq. (4.15). These rotations correspond to rearranging the order in which the different particles are grouped together, and therefore link different partition chains. A useful set of transformations is formed by $P^\pm$ and $Q^\pm$, which are just special cases of the transformation (4.15), and a simple reflection operator $P_y$:

\begin{align}
P^+ \{x, y, z\}_{(ijk)l,(ij)kl} &= \{x, y, z\}_{(klj)l,(kl)ji}, \quad (7.7a) \\
P^- \{x, y, z\}_{(ijk)l,(ij)kl} &= \{x, y, z\}_{(jki)l,(jk)il}, \quad (7.7b) \\
Q^+ \{x, y, z\}_{(ijk)l,(ij)kl} &= \{x, y, -z\}_{(ijk)(kl),(ij)ki}, \quad (7.7c) \\
Q^- \{x, y, z\}_{(ijk)l,(ij)kl} &= \{x, -y, z\}_{(ijl)k,(ijkl)k}, \quad (7.7d) \\
Q^+ \{x, y, -z\}_{(ijk)l,(ij)kl} &= \{x, -y, z\}_{(ijkl)k,(ijkl)k}, \quad (7.7e) \\
Q^- \{x, y, -z\}_{(ijk)l,(ij)kl} &= \{x, y, z\}_{(ijkl),(ijkl)k}, \quad (7.7f) \\
P_y \{x, y, z\}_{(ijkl),(ij)kl} &= \{x, y, z\}_{(kl)ij,(kl)ij}. \quad (7.7g)
\end{align}

The transformations used in the Yakubovsky equations can be constructed as follows:

\begin{align}
P^+ \{x, y, z\}_{(ijk)l,(ij)kl} &= \{x, y, z\}_{(klj)l,(kl)ji}, \quad (7.8a) \\
P^- \{x, y, z\}_{(ijk)l,(ij)kl} &= \{x, y, z\}_{(jki)l,(jk)il}, \quad (7.8b) \\
Q^- P^+ \{x, y, z\}_{(ijk)l,(ij)kl} &= \{x, -y, z\}_{(kli)j,(kij)ji}, \quad (7.8c) \\
Q^- P^- \{x, y, z\}_{(ijk)l,(ij)kl} &= \{x, -y, z\}_{(ijkl)k,(ijkl)k}, \quad (7.8d) \\
Q^+ P^+ \{x, y, z\}_{(ijkl),(ij)kl} &= \{x, y, -z\}_{(ij)j,(ij)j}, \quad (7.8e) \\
Q^+ P^- \{x, y, z\}_{(ijkl),(ij)kl} &= \{x, y, -z\}_{(ijkl),(ijkl)k}, \quad (7.8f) \\
P_y \{x, y, z\}_{(ijkl),(ij)kl} &= \{x, y, z\}_{(kji)(ij)}, \quad (7.8g) \\
Q^+ P_y \{x, y, -z\}_{(ijkl),(ij)kl} &= \{x, -y, z\}_{(klj)k,(klj)k}, \quad (7.8h) \\
Q^- P_y \{x, y, -z\}_{(ijkl),(ij)kl} &= \{x, y, z\}_{(klj)k,(klj)k}. \quad (7.8i)
\end{align}

The transformations $P^\pm$ are identical to the transformations used in the three-body problem (i.e., the fourth particle is simply disregarded), whereas the transformations $Q^\pm$ treat the pair $(ij)$ as a single fragment of a three-fragment system. The operator $P_y$ interchanges the two two-particle fragments. (When constructing the total wave function all eighteen amplitudes are necessary, and all possible
transformations are needed. Apart from reflections, these transformations involve products of at most three of the basic transformations \( P^\pm \) and \( Q^\pm \). Note that in Merkuriev and Yakovlev [1984] different transformations were defined which have the disadvantage that some of them transform all three Jacobi coordinates, and are therefore inefficient from a numerical point of view. (This will be explained later on.)

### 7.2.1 Partial-wave analysis

In order to reduce the number of continuous variables in the equations, we expand the Yakubovsky amplitudes on a tripolar basis:

\[
\psi_a(x, y, z) = \sum_{\alpha} \frac{\psi_\alpha^a(x, y, z)}{\alpha} \alpha(\hat{x}, \hat{y}, \hat{z}). \tag{7.9}
\]

Here \( \alpha(\hat{x}, \hat{y}, \hat{z}) \) is a tripolar harmonic, which can be constructed using spherical and bipolar harmonics:

\[
\alpha(\hat{x}, \hat{y}, \hat{z}) = \left[ [Y_{\ell_a}(\hat{x}) \otimes Y_{\ell'_a}(\hat{y})]_{L_\alpha} \otimes Y_{\ell''_a}(\hat{z}) \right]_{L_\alpha M_\alpha} = \sum_{m, m'} \langle L'_\alpha m | L_{\alpha} M_\alpha \rangle [Y_{\ell_a}(\hat{x}) \otimes Y_{\ell'_a}(\hat{y})]_{L'_\alpha m} Y_{\ell''_a}(\hat{z}). \tag{7.10}
\]

After projecting out a particular angular-momentum state \( \alpha \) and after inserting unit operators of the form \( \int \text{d}x' \text{d}y' \text{d}z' \left[ x' y' z' \right] \langle x' y' z' | x, y, z \rangle \), we find the following equations:

\[
[E - H_{0,a}^\alpha - V_a(x)] \psi_\alpha^a(x, y, z) = V_a(x) \frac{1}{2L + 1} \sum_{M} \sum_{b} \sum_{\beta} \int \text{d}x \text{d}y \text{d}z K_{ab}^{\alpha\beta}(x, y, z) \psi_\beta^b(x, y, z), \tag{7.11}
\]

with

\[
H_{0,a}^\alpha = -\frac{\partial^2}{\partial x^2} + \frac{\ell_a(\ell_a + 1)}{x^2} - \frac{\partial^2}{\partial y^2} + \frac{\ell'_a(\ell'_a + 1)}{y^2} - \frac{\partial^2}{\partial z^2} + \frac{\ell''_a(\ell''_a + 1)}{z^2}. \tag{7.12}
\]

For the bound-state case the boundary conditions are clearly

\[
0 = \psi_\alpha^a(0, y, z) = \psi_\alpha^a(x, 0, z) = \psi_\alpha^a(x, y, 0)
\]

\[
= \psi_\alpha^a(\infty, y, z) = \psi_\alpha^a(x, \infty, z) = \psi_\alpha^a(x, y, \infty). \tag{7.13}
\]

The kernel \( K_{ab}^{\alpha\beta} \) is the generalization of the kernel \( K_{ij}^{\alpha\beta} \) for the three-body system. It can be written as

\[
K_{ab}^{\alpha\beta}(x_a, y_a, z_a) = \frac{x_a y_a z_a}{x_b y_b z_b} \alpha^*(\hat{x}_a, \hat{y}_a, \hat{z}_a) \beta(\hat{x}_b, \hat{y}_b, \hat{z}_b), \tag{7.14}
\]
7.2 Coordinates in the four-body system

where $\alpha(\hat{x}, \hat{y}, \hat{z})$ and $\beta(\hat{x}, \hat{y}, \hat{z})$ are tripolar harmonics, and the sum is over all chains which do not have the same three-fragment partition as $a$. Note that $\{x, y, z\}_b$ is a function of $\{x, y, z\}_a$. The kernel $K^{\alpha\beta}_{ab}$ is a function of three vectors, and therefore a complicated object. However, by inserting unit operators $\int da'' \, dy'' \, dz'' \, |x'' \, y'' \, z''\rangle_c \langle x'' \, y'' \, z''|$, where $c$ is an “intermediate” coordinate system (i.e., a coordinate system which can be transformed into both $a$ and $b$ by just one operator $P^\pm$, $Q^\pm$ or $P_y$), the kernel can be factorized into simpler objects. These objects are of course just special cases of $K^{\alpha\beta}_{ab}$. Since $P^\pm$, $Q^\pm$, and $P_y$ leave at least one variable unaffected, the first of the three angular integrations is trivial. A second can be performed simply by observing that the kernel only depends on the angle between the two vectors that are being transformed (i.e., on $\hat{x} \cdot \hat{y}$ or $\hat{y} \cdot \hat{z}$). In the next section the evaluation of these integrals will be discussed in more detail.

7.2.2 Evaluation of the integrals

As was shown in Sec. 7.2, the transformations relating the various coordinate systems can be written as products of a few basic transformations, four of which are nontrivial. These basic transformations will be discussed first. After that, the basic transformations will be combined to generate all the possible transformations.

In analogy to the approach used in the three-body problem, we introduce spherical coordinates to denote the lengths of the vectors $x$, $y$, and $z$:

\begin{align}
    x &= \rho \sin \phi \cos \theta, \\
    y &= \rho \sin \phi \sin \theta, \\
    z &= \rho \cos \phi.
\end{align}

As in the three-body case, the hyperradius $\rho$ is independent of the coordinate system.

First, we consider a transformation $P$, defined by

\[
\begin{pmatrix}
    x' \\
    y'
\end{pmatrix} = \begin{pmatrix}
    -\cos \mu & \sin \mu \\
    -\sin \mu & -\cos \mu
\end{pmatrix} \begin{pmatrix}
    x \\
    y
\end{pmatrix},
\]

where $\mu$ may be any angle. Note that $x^2 + y^2$ is left invariant by this transformation, and it is therefore sufficient to describe the relation between the angles $\theta$ and $\theta'$. This relation can be written as follows:

\[
\cos^2 \theta' = \cos^2 \mu \cos^2 \theta + \sin^2 \mu \sin^2 \theta - 2 \hat{x} \cdot \hat{y} \sin \mu \cos \mu \sin \theta \cos \theta.
\]

Clearly, the only nontrivial dependence on the directions of $x$, $y$, and $z$ is the angle between $x$ and $y$. The coordinate transformation applied to an amplitude
\[\psi_b\] can be expressed as

\[
\frac{1}{2L+1} \sum_M \int d\hat{x} d\hat{y} d\hat{z} \frac{x'y'}{x'y'} \alpha^*(\hat{x}, \hat{y}, \hat{z}) \beta(\hat{x}', \hat{y}', \hat{z}') \psi_b^\beta(x', y', z)
\]

\[= \frac{16\pi^2}{\sin 2|\mu|(2L+1)} \sum_M \int d\theta' \psi_b^\beta(\rho, \theta', \phi) \int d\hat{z} \alpha^*(\hat{x}, \hat{y}, \hat{z}) \beta(\hat{x}', \hat{y}', \hat{z})
\]

\[= \int d\theta' P_{a'b}^{\alpha\beta}(\theta, \theta') \psi_b^\beta(\rho, \theta', \phi), \quad (7.18)
\]

where the freedom to choose \(\hat{y}\) to lie along the \(\hat{e}_z\) axis along and to choose \(\hat{x}\) to lie in the \(\hat{e}_x-\hat{e}_z\) plane was used. This leaves just the integration over \(\hat{z}\) and the integration over \(\hat{x} \cdot \hat{y}\). Note that a change of integration variable from \(d\hat{x} \cdot \hat{y}\) to \(d\theta'\) was made. The kernel \(P_{a'b}^{\alpha\beta}\) is just the kernel \(K_{ij}^{\alpha\beta}\) of Eq. (5.9), embedded in the space of three angular variables.

The integration limits can be obtained by substituting the extreme values for \(\hat{x} \cdot \hat{y}\) in Eq. (7.17):

\[|\theta - |\mu|| \leq \theta' \leq \pi - |\theta - |\mu||. \quad (7.19)
\]

The above formulas are essentially equal to the formulas for the three-body case, as was to be expected.

Less convenient is the transformation \(Q\), defined by

\[
\left(\begin{array}{c}
y' \\
z'
\end{array}\right) = \left(\begin{array}{cc}
\cos \mu & \sin \mu \\
-\sin \mu & \cos \mu
\end{array}\right) \left(\begin{array}{c}
y \\
z
\end{array}\right),
\]

\[\quad \text{where } \mu \text{ may be any angle. (Note that a convenient but nonessential reflection was introduced in the transformation matrix.) This leads to the following expression for } \cos^2 \phi':
\]

\[\cos^2 \phi' = \sin^2 \mu \sin^2 \phi \sin^2 \theta + \cos^2 \mu \cos^2 \phi
\]

\[\quad - 2 \hat{y} \cdot \hat{z} \sin \mu \cos \mu \sin \phi \sin \theta \cos \phi. \quad (7.21)
\]

From the fact that \(x\) remains unchanged, it follows that

\[\cos \theta' = \frac{\sin \phi \cos \theta}{\sin \phi'}. \quad (7.22)
\]

These expressions lead to

\[
\frac{1}{2L+1} \sum_M \int d\hat{x} d\hat{y} d\hat{z} \frac{y'z'}{y'z'} \alpha^*(\hat{x}, \hat{y}, \hat{z}) \beta(\hat{x}', \hat{y}', \hat{z}') \psi_b^\beta(x, y', z')
\]

\[= \frac{16\pi^2}{\sin 2|\mu|} \int \frac{d\phi'}{\sin \theta'} \psi_b^\beta(\rho, \theta', \phi') \int d\hat{x} \alpha^*(\hat{x}, \hat{y}, \hat{z}) \beta(\hat{x}', \hat{y}', \hat{z}')
\]

\[= \int d\phi' Q_{a'b}^{\alpha\beta}(\theta, \phi, \phi') \psi_b^\beta(\rho, \theta', \phi'). \quad (7.23)
\]
The integration limits for Eq. (7.23) are a little more intricate than for the previous case:

\[
|\sin |\mu| \sin \phi \sin \theta - \cos |\mu| \cos \phi| \\
\leq \cos \phi' \\
\leq |\sin |\mu| \sin \phi \sin \theta + \cos |\mu| \cos \phi| .
\] (7.24)

Note that the integration kernel \( Q_{\alpha \beta}^{ab} \) depends on three variables, and is therefore a much more complicated object than \( P_{\alpha \beta}^{ab} \) which depends on two variables. Fortunately, it contains a factor \( \delta_{\epsilon_a \epsilon_b} \), so that the number of nonzero blocks is relatively small.

Products of various coordinate transformations can be written as products of integral kernels. Let us consider as an example the evaluation of \( \psi_{(k)i,l,(k)i,lj} \) in the natural coordinate system of \( \psi_{(ij)(i,l),(k)i,j} \). (Note that the equation for \( \psi_{(ijk)(ij),(k)kl} \) contains \( \psi_{(kii),(k)i,j} \) on the right-hand side.) According to Eq. (7.8c) these two coordinate systems are related by the operator \( Q^- P^+ \), which can be written in the following form:

\[
(\text{ijkl},(ij)kl) (x,y,z) \alpha \left| \psi_{(kii),(k)i,j} \right|^\beta \\
= \sum_\gamma \int d\theta' P^{\alpha \gamma}_{\{ijkl\},\{ij\}kl} \{\{kii\},\{iji\}\} (\theta, \theta') \\
\times \int d\phi' Q^{\gamma \beta}_{\{kii\},\{kii\}ij} \{\{kii\},\{kii\}ij\} (\theta', \phi', \phi') \psi_{b}^_tail(\rho, \theta'', \phi'),
\] (7.25)

where \( \theta'' \) is a function of \( \theta' \), \( \phi' \), and \( \phi'' \). Equation (7.25) illustrates how products of the four basic transformations can be used to generate all necessary transformations.

### 7.2.3 Identical particles

If some of the particles are indistinguishable, the Yakubovsky equations can be simplified significantly. Suppose, for example, that particles \( i \) and \( j \) are identical. This implies that a partition chain \( a \) related to another chain \( b \) in the sense that it becomes \( b \) if particle labels \( i \) and \( j \) are interchanged (e.g., the coordinate system labeled by \( \{(k)ij\},\{(k)lj\} \) is related to the one labeled by \( \{(k)il\},\{(k)lj\} \) by interchange of \( i \) and \( j \)) can be considered identical to \( b \) provided particles \( i \) and \( j \) may be interchanged, i.e., if they are indistinguishable.

It is easy to show that this symmetry has important consequences for the Faddeev and Yakubovsky components:

\[
P_{ij} \psi_{a_3} = p \psi_{a_3} ,
\] (7.26)
\[
P_{ij} \psi_{a_3} = p \psi_{a_3} ,
\] (7.27)
Table 7.1: Possible symmetries in the four-body system.

<table>
<thead>
<tr>
<th></th>
<th>1111</th>
<th>211</th>
<th>22</th>
<th>31</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Faddeev</td>
<td>6</td>
<td>4</td>
<td>3</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>Yakubovsky</td>
<td>12 + 6</td>
<td>7 + 4</td>
<td>4 + 3</td>
<td>3 + 2</td>
<td>1 + 1</td>
</tr>
</tbody>
</table>

where $p$ is $\pm$ depending on the spin of the particles $i$ and $j$. These equalities imply a reduction from six to four Faddeev components, and a reduction from $12 + 6$ to $7 + 4$ Yakubovsky components.

Table 7.1 lists all the possible symmetries, and the number of independent components. For the remainder of this chapter all particles will be assumed to be identical, so that there are just two independent Yakubovsky components. Note that in the case of identical particles, the coordinate transformations defined in Sec. 7.2 have a one-to-one correspondence to specific permutations of the particles, and that the integral kernels associated with these coordinate transformations can be seen as the configuration-space representations of the corresponding permutation operators.

### 7.3 Numerical solution

The numerical solution methods that were used by Schut to solve the four-body problem are, apart from the clearly much larger demand on computer capacity, very similar to those used in the three-body problem. In this section I will describe the extension of the spline method to the four-body problem, as well as the factorization and numerical solution of the resulting matrix equation.

#### 7.3.1 Discretization

The spherical coordinates described by Eq. (7.15) and the transformation

$$\tilde{\rho} = 1 - e^{-\lambda \rho},$$

where $\lambda$ is an adjustable (positive) constant, can be used to cast the four-body Yakubovsky equations (7.11) in a convenient form. The result can be written as follows:

$$[E - H_{0,a}^\alpha - V_a(\rho(\tilde{\rho}) \sin \phi \cos \theta)]\psi_a^\alpha(\tilde{\rho}, \theta, \phi)$$

$$= V_a(\rho(\tilde{\rho}) \sin \phi \cos \theta)$$

$$\times \frac{1}{2L + 1} \sum_M \sum_b \sum_\beta \int d\theta' d\phi' K_{0,a}^{\alpha\beta}(\theta, \phi, \theta', \phi') \psi_b^\beta(\tilde{\rho}, \theta', \phi'),$$

Equation (7.29)
with
\[ H_{\alpha,\alpha}^\beta = -\lambda^2(1 - \bar{\rho})^2 \frac{\partial^2}{\partial \bar{\rho}^2} + \lambda(1 - \bar{\rho}) \left( \lambda - \frac{2}{\rho(\bar{\rho})} \right) \frac{\partial}{\partial \bar{\rho}} \]
\[ - \frac{1}{\rho^2(\bar{\rho})} \left\{ \frac{\partial^2}{\partial \phi^2} + \cot \phi \frac{\partial}{\partial \phi} + \frac{1}{\sin^2 \phi} \frac{\partial^2}{\partial \theta^2} \right\} \]
\[ + \frac{1}{\rho^2(\bar{\rho})} \left\{ \ell_\alpha(\ell_\alpha + 1) \left( \frac{\ell'_\alpha(\ell'_\alpha + 1)}{(\sin \phi \cos \theta)^2} + \frac{\ell''_\alpha(\ell''_\alpha + 1)}{(\sin \phi \sin \theta)^2} \right) \right\}. \tag{7.30} \]

The boundary conditions are:
\[ 0 = \psi_{\alpha}^\gamma(0, \theta, \phi) = \psi_{\alpha}^\gamma(\bar{\rho}, 0, \phi) = \psi_{\alpha}^\gamma(\bar{\rho}, \theta, 0) \]
\[ = \psi_{\alpha}^\gamma(1, \theta, \phi) = \psi_{\alpha}^\gamma(\bar{\rho}, \frac{\pi}{2}, \phi) = \psi_{\alpha}^\gamma(\bar{\rho}, \theta, \frac{\pi}{2}). \tag{7.31} \]

Now the Yakubovsky amplitudes are approximated by a tricubic spline expansion:
\[ \psi_{\alpha}^\gamma(\bar{\rho}, \theta, \phi) \approx \sum_{ijk} \psi_{ijk}^\gamma s_i(\bar{\rho}) s_j(\theta) s_k(\phi), \tag{7.32} \]
where \( \psi_{ijk}^\gamma \) are expansion coefficients, where the spline functions \( s_i \) form a basis set on a grid subdividing \([0,1]\) into \( N_\rho \) intervals, satisfying the correct boundary conditions, and where \( s_j \) and \( s_k \) form basis sets on grids subdividing \([0, \frac{\pi}{2}]\) into \( N_\theta \) and \( N_\phi \) intervals, respectively, also satisfying the appropriate boundary conditions.

Collocating in the \( 2 \times 2 \times 2 \) Gauss points for every interval on the three-dimensional grid leads to the following equation:
\[ (EI - T - V)\psi = P\psi, \tag{7.33} \]
where \( E \) is the (energy) eigenvalue, \( \psi \) is the vector of expansion coefficients \( \psi_{mn}^{\alpha,\gamma} \), and \( I, T, V, \) and \( P \) are \( 2N_\rho 2N_\theta 2N_\phi N_c \times 2N_\rho 2N_\theta 2N_\phi N_c \) matrices, whose matrix elements are:
\[ I_{pqr,mn}^{\alpha,\beta} = \delta_{\alpha,\beta} s_m(\bar{\rho}_p) s_n(\theta_q) s_o(\phi_r), \tag{7.34a} \]
\[ T_{pqr,mn}^{\alpha,\beta} = \delta_{\alpha,\beta} \left[ T_{p,m}^{\phi} s_n(\theta_q) s_o(\phi_r) \right. \]
\[ + \left. \frac{1}{\rho^2(\bar{\rho}_p)} s_m(\bar{\rho}_p) \left( T_{o,r}^{\phi} s_n(\theta_q) + \frac{1}{\sin^2 \phi_r} s_o(\phi_r) T_{n,q}^{\theta} \right) \right], \tag{7.34b} \]
\[ V_{pqr,mn}^{\alpha,\beta} = V_{\alpha,\beta}^{\gamma} (\rho(\bar{\rho}_p) \cos \theta_q \sin \phi_r) s_m(\bar{\rho}_p) s_n(\theta_q) s_o(\phi_q), \tag{7.34c} \]
\[ P_{pqr,mn}^{\alpha,\beta} = \sum_{\gamma} V_{\alpha,\beta}^{\gamma} \left( \rho(\bar{\rho}_p) \cos \theta_q \sin \phi_r \right) s_m(\bar{\rho}_p) \]
\[ \times \int d\theta d\phi K_{\alpha,\beta}^{\gamma} \left( \theta_q, \phi_r, \theta, \phi \right) s_n(\theta) s_o(\phi), \tag{7.34d} \]
with
\[
T_{p,m}^\rho = -\lambda^2 (1 - \bar{\rho}_p^2) s_m' (\bar{\rho}_p) + \lambda (1 - \bar{\rho}_p) \left( \lambda - \frac{2}{\rho(\bar{\rho}_p)} \right) s_m' (\bar{\rho}_p),
\]
\[
T_{q,n}^\theta = -s_m'' (\theta_q) + \frac{\ell_\alpha (\ell_\alpha + 1)}{\cos \theta_q^2} s_n (\theta_q) + \frac{\ell_\alpha' (\ell_\alpha' + 1)}{\sin \theta_q^2} s_n (\theta_q),
\]
\[
T_{r,o}^\phi = -s_m'' (\phi_r) - \cot \phi_r s_m' (\phi_r) + \frac{\ell_\alpha' (\ell_\alpha' + 1)}{\cos \phi_r^2} s_m (\phi_r).
\]
(Equations (7.35), (7.36), and (7.37) describe the matrix elements of smaller matrices, which I will denote by \(T_{p,m}, T_{q,n},\) and \(T_{r,o},\) respectively.) Note that the matrix \(I\) can be seen as the spline representation of the unit operator, \(T\) is the kinetic energy operator, \(V\) the potential, and \(P\) is the operator on the right-hand side of the Yakubovsky equations, containing the potentials and the integrals. Note also that the potential was allowed to be nondiagonal in the channel space. I will now proceed by describing the solution of the eigenvalue equation (7.33).

### 7.3.2 Solution of the matrix problem

The matrix equation for the discretized four-body problem, Eq. (7.33), bears a great resemblance to the matrix equation for the three-body problem in polar coordinates. The difference is that there are now three types of spline matrices, instead of two, and that the integral operators are more involved as compared to the three-body integral operators. Considering the fact that again, it is practically impossible to invert the right-hand side of Eq. (7.33), and that again, the spectrum makes it difficult to find the energy eigenvalue iteratively, it is useful to proceed in a way similar as described in Chapter 5: transfer all the potential terms to the right-hand side, substitute an estimate of the energy eigenvalue, invert the left-hand side, and introduce a new eigenvalue \(\Lambda:\)

\[
(E_0 I - T)^{-1} (P + V) \psi = \Lambda \psi.
\]

The inverse of \(E_0 I - T\) can be calculated efficiently by using a trick similar to the one described in Sec. 5.3.6: \(E_0 I - T\) can be written as

\[
\tilde{T}_\rho \otimes S_\phi \otimes S_\theta + R_\rho \otimes (T_\phi \otimes S_\theta + R_\phi \otimes T_\theta)
= (\tilde{R}_\rho \otimes 1 \otimes 1)(\tilde{R}_\rho^{-1} T_\phi \otimes S_\theta + 1 \otimes (T_\phi \otimes S_\theta + R_\phi \otimes T_\theta))
= (\tilde{R}_\rho U_\rho^{-1} \otimes 1 \otimes 1) [\Gamma_\rho \otimes S_\phi \otimes S_\theta + 1 \otimes (T_\phi \otimes S_\theta + R_\phi \otimes T_\theta)]
= (U_\rho \otimes 1 \otimes 1),
\]

where \(\tilde{T}_\rho\) is defined as \(T_\rho - E_0 S_\rho,\) \(\Gamma_\rho\) is diagonal, satisfying \(\tilde{R}_\rho^{-1} T_\rho = U_\rho^{-1} \Gamma_\rho U_\rho,\) and

\[
R_{m,p}^\rho = \frac{1}{\rho^2 (\bar{\rho}_p)} s_m (\bar{\rho}_p),
\]
\[ R_{\alpha,r}^{\phi} = \frac{1}{\sin^2 \phi_r} s_\theta(\phi_r). \] (7.41)

Equation (7.39) can be regarded as a product of two fully factorized matrices (first and last factor), and of a matrix which is diagonal in \( \bar{\rho} \) space, the elements of which are

\[ \gamma_S S_{\phi} \otimes S_{\theta} + (T_{\phi} \otimes S_{\theta} + R_{\phi} \otimes T_{\theta}) = (\gamma_S S_{\phi} + T_{\phi}) \otimes S_{\theta} + R_{\phi} \otimes T_{\theta}, \] (7.42)

This can be written as a product of fully factorized matrices, and a diagonal nonfactorizable matrix using the trick of Chapter 5. The inverse of \( E_0 I - T \) can therefore be written as a product of two completely factorized matrices, and a third, which is diagonal in \( \bar{\rho} \) space and which has elements which are products of factorized matrices and a diagonal matrix.

If, for the sake of simplicity, we assume that all grids have \( N \) intervals, the amount of storage needed to store the matrix representing the inverse of \( E_0 I - T \) is \( O(N^3 N_c) \). The computer time needed to calculate the inverse is \( O(N^4 N_c) \), which is also the time needed to multiply this matrix with a vector. This method requires therefore only \( N \) times more computer memory and time for the four-body problem than is required for the three-body problem. (Note, however, that for the four-body problem, the number of channels \( N_c \) is in general much larger than for the three-body problem.)

The remaining question is how to implement the right-hand side of Eq. (7.38) efficiently. The key to answering this lies in the separation of the coordinate transformations into simple rotations which involve at most two variables, as described by Eq. (7.25). Using the spline method, this can be implemented as follows. First, rewrite the right-hand side as

\[ P = V \left[ 1_\rho \otimes \left( \sum_{ab} S^{-1} P_{ab} + \sum_{abc} S^{-1} P_{ac} S^{-1} P_{cb} \right) \right], \] (7.43)

with

\[ [P_{ab}]_{\alpha',\beta'}^{\alpha,\beta} = \delta_{\alpha,\alpha'} \delta_{\beta,\beta'} \int d\theta d\phi K_{\alpha,\beta}^{\alpha',\beta'}(\theta, \phi_r, \theta, \phi) s_n(\theta) s_\theta(\phi), \] (7.44)

\[ S_{\alpha,\beta}^{\alpha',\beta'} = \delta_{\alpha,\alpha'} \delta_{\beta,\beta'} s_n(\theta) s_\theta(\phi_r), \] (7.45)

where in this case Eq. (7.45) is only defined if \( \alpha \) and \( \beta \) are related by a single simple coordinate transformation (\( i.e., P^\pm, Q^\pm, \text{ or } P_y \)). Note that the sums in Eq. (7.43) are to be taken such that only these terms occur.

The spline representations of the simple transformations are

\[ [P_{ab}]_{\alpha',\beta'}^{\alpha,\beta} = \delta_{\alpha,\alpha'} \delta_{\beta,\beta'} s_\theta(\phi_r) \int d\theta K^{\alpha,\beta}_{\alpha',\beta'}(\theta, \phi_r) s_n(\theta), \] (7.46)
for $P^\pm$,

$$[P_{ab}]_{q,r,n_o}^{\alpha_a \beta_b} = \delta_{a,a'} \delta_{b,b'} \int d\phi K_{ab}^{\alpha_a \beta_b} (\theta_q, \phi_r, \phi) s_n(\theta) s_o(\phi), \quad (7.47)$$

for $Q^\pm$, and

$$[P_{ab}]_{q,r,n_o}^{\alpha_a' \beta_b'} = \delta_{a,a'} \delta_{b,b'} \delta_{\alpha_a, \beta_b} s_{\alpha, \beta}(\pi/2 - \theta_q) s_o(\phi_r), \quad (7.48)$$

for $P_y$. (Note that $\delta_{\alpha_a, \beta_b}$ was written to denote that the angular-momentum state $\alpha_a$ should be identical to the state obtained by interchanging the quantum numbers associated with $x$ and $y$ of angular-momentum state $\beta_b$.)

The matrices for $P^\pm$ and $P_y$ can immediately be factorized, but the matrix corresponding to $Q^\pm$ cannot. However, since there is fixed relation between $\phi$ and $\theta$ (cf. Eq. (7.22)) as a function of $\theta_q$ and $\phi_r$, only a small number of elements is nonzero: for every pair of collocation points $\theta_q$ and $\phi_r$ there is a (curved) integration path in the plane $(\theta, \phi)$, to which only $O(N)$ spline functions contribute. This matrix can therefore be stored as a sparse matrix, requiring $O(N^3 N^2)$ elements.

### 7.4 Results

This section discusses some results that were obtained with the method described in this chapter. Note that the numerical calculations were done by Schut. As a numerical test, the ground state of four identical particles interacting via harmonic oscillator potentials was calculated. In a first publication, several s-wave spin-independent and spin-dependent potentials were used [Schellingerhout et al., 1992]. The ultimate object was to calculate the four-nucleon bound state, but at the time of writing this thesis, this project was not yet completed. However, the first step—including higher partial waves—was made [Schellingerhout et al., 1993].

#### 7.4.1 Harmonic oscillator

Since the harmonic oscillator can be solved exactly for any $N$-body system, it can be used as an initial numerical test. The four-body ground-state energy was calculated using the harmonic oscillator with a cutoff at $r = 5$ (cf. Appendix B). In Table 7.2 the convergence of the eigenvalue $\Lambda$ is shown. The extrapolated result is $E_0 = -\sqrt{2} \cdot 8.99999(3)$, which is in excellent agreement with exact value of $-9\sqrt{2}$. Note that the derivative $dE_0/d\Lambda$ is a measure for the potential energy. Correcting for the offset of $-150$ due to the way in which the harmonic oscillator was modeled, this derivative is found to be approximately $6.365$ (using the values for fourteen intervals) or $\sqrt{2} \cdot 4.5007 \ldots$, which is also in good agreement with theory. (This value should not be taken too seriously, since the Lanczos process was broken off after a very small number of steps, and the derivative was calculated using two trial energies that were extremely close. There is no guarantee that the eigenvalues
Table 7.2: Eigenvalues for the harmonic-oscillator four-body problem, with $E_0 = -137.2721$. (The theoretical ground-state energy is $9\sqrt{2} - 150 = -137.27207\ldots$)

<table>
<thead>
<tr>
<th>$N_\rho$</th>
<th>$N_\theta$</th>
<th>$N_\phi$</th>
<th>$\Lambda$</th>
<th>$dE_0/d\Lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>7</td>
<td>7</td>
<td>0.99992679</td>
<td>-143.621</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>10</td>
<td>1.00002381</td>
<td>-143.638</td>
</tr>
<tr>
<td>14</td>
<td>14</td>
<td>14</td>
<td>1.00000437</td>
<td>-143.635</td>
</tr>
<tr>
<td>20</td>
<td>20</td>
<td>20</td>
<td>1.00000126</td>
<td>-146.124</td>
</tr>
<tr>
<td>28</td>
<td>28</td>
<td>28</td>
<td>1.00000041</td>
<td>-132.647</td>
</tr>
</tbody>
</table>
| $\infty$ | $\infty$  | $\infty$| 1.0000001(2) |}

have converged sufficiently far to warrant all digits shown for the derivative. This is clearly illustrated by the results for more than fourteen intervals, where the convergence of the Lanczosos process is slightly slower, and therefore the derivative is less reliable. The errors in the eigenvalues $\Lambda$ are smaller than 1 in the last digit.

Note that all orbital angular momenta were taken to be zero here (i.e., $\ell = \ell' = \ell'' = 0$). Unlike the three-body case, this is not equivalent to using an s-wave projected potential: there is an infinite number of states with $\ell = 0$. Also, since the coordinate transformations are performed in two steps, there is an additional approximation: the intermediate amplitude is projected on this partial-wave state. Since the ground-state of the harmonic oscillator is symmetric in all interparticle distances, its only nonzero partial wave is $\ell = \ell' = \ell'' = 0$. It is not immediately clear that this should be true for the Yakubovsky amplitudes as well, but we may conclude that the other partial waves, if present, are negligibly small.

7.4.2 s-wave potentials

Since four-body calculations require an enormous numerical effort, most calculations have been performed using very simple interaction models, including at best just a spin dependence. The simplest models are purely central or even s-wave projected. In Table 7.3 an overview of results for s-wave projected potentials is given. The results are ordered chronologically. The first result, denoted by HSE (short for Hilbert–Schmidt expansion) is taken from Tjon [1975]. It was the first attempt at solving the Yakubovsky equations in momentum space non-variationally. The three-dimensional integral equations were reduced to a set of one-dimensional integral equation by using two consecutive separable expansions.\(^2\)

\(^2\)There is much confusion around the Malffiet–Tjon potentials. The potential MT-I/IIIa was refitted by Payne et al. [1980] in order to reproduce the deuteron binding energy, since the original potential gives too much binding. A possible explanation of the discrepancy is given in Appendix B. It is possible that Tjon actually used the potential MT-I/IIIc, described there.
Table 7.3: Overview of literature values of four-body ground-state energies $E_0$ and comparison with present calculations for various simple nuclear potentials. See text for explanation of the methods and references.

<table>
<thead>
<tr>
<th>Method</th>
<th>MT-Vb</th>
<th>MT-V</th>
<th>S3</th>
<th>MT-I/III</th>
</tr>
</thead>
<tbody>
<tr>
<td>HSE</td>
<td></td>
<td></td>
<td></td>
<td>29.6(2)</td>
</tr>
<tr>
<td>SPE</td>
<td></td>
<td></td>
<td></td>
<td>30.36</td>
</tr>
<tr>
<td>YDE</td>
<td>29.1(2)</td>
<td>25.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SIDE</td>
<td>28.47</td>
<td>29.74</td>
<td>25.38</td>
<td>29.74</td>
</tr>
<tr>
<td>YIE</td>
<td>28.83</td>
<td>30.07</td>
<td>25.69</td>
<td>30.29</td>
</tr>
<tr>
<td>YDE(1)</td>
<td>28.7808(2)</td>
<td>30.0628(2)</td>
<td>25.6745(3)</td>
<td>30.3117(3)</td>
</tr>
<tr>
<td>YDE(2)</td>
<td></td>
<td>30.0634(5)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A similar method was later applied by Sofianos et al. [1982]. (This result is denoted by SPE: separable pole expansion.) Due to the nonsystematic convergence of separable expansions, it is very difficult to give error estimates for these results.

A first attempt at solving the Yakubovsky differential equations exactly made by Merkuriev et al. [1984]. Their calculations appear to be accurate to within a few hundred keV. A radically different approach, known as IDEA, is to reformulate the $N$-body equations and to take only two-body correlations into account [Oehm et al., 1990]. The $s$-wave version of this approach, SIDE, gives a few hundred keV less binding than the exact value, indicating that this approximation works fairly well. Its disadvantage is of course, that the result cannot be improved without drastically complicating the equations. The first numerically and technically essentially exact calculations are those by Schellinghout et al. [1992] (denoted by YDE(1) and YDE(2); for a discussion of the details on grid parameters, see Schellinghout et al. [1992]) and Kamada and Glöckle [1992] (denote by YIE: Yakubovsky integral equations). The agreement between these calculations is excellent (typically on the order of 10 keV), indicating that finally numerical technique has advanced to a level where it becomes possible to investigate “small” effects reliably.

A few final remarks are in order. The difference between YDE(1) and YDE(2) is that in YDE(1) only one channel was taken into account, whereas in YDE(2) $\ell'$ and $\ell''$ were allowed to be greater than zero (but smaller than or equal to four). The effect of these extra partial waves is negligible. However, it should be noted that even YDE(2) is not a complete $s$-wave calculation, since the coordinate transformations that consist of two steps have an additional projection, as discussed earlier. It is difficult to estimate the error introduced by this approximation, but
since it involves a coupling from $\ell = 0$ to $\ell \neq 0$ and another one from $\ell \neq 0$ to $\ell = 0$, it is “of second order,” and can therefore be expected to be much smaller than the effect of including all partial waves throughout the equations (which is of the order of one MeV; see below). Note that Kamada and Glöckle [1992] perform the coordinate transformations in a similar manner, and therefore make a similar approximation.

### 7.4.3 Higher partial waves

When the restriction to $s$-wave interactions is released, the binding energy increases by approximately one MeV. This is illustrated for the MT-V potential in Table 7.4. In this table the results obtained by Schut, using the methods described in this chapter (YDE [Schellinghout, 1994]) and the results of Kamada and Glöckle [1992] are compared. The agreement is near perfect in all cases. From the convergence behavior of the partial-wave series one can infer that the full result is $E = -31.339(5)$ MeV.

Note that the partial-wave series converges very quickly, and the convergence is very similar to the convergence that was observed for the corresponding three-body case. (The relative error in the binding energy is of the same order as for the three-body case, if the potential is cut off at the same angular momentum; cf. Table 5.5.) Note also, that the cutoff in the $x$ variable is most important. (Cutting off $\ell_z$ at a specific value leads to an error which is approximately one order of a magnitude smaller than the error corresponding to a similar cutoff for $\ell_x$.) This was to be expected, since the Yakubovsky components have the most structure in the $x$ variable.

### 7.4.4 Comparison with the literature

The first practical calculations of the four-nucleon bound state were of a variational nature. Two examples of such calculations can be found in Tang et al. [1965] and Fantoni et al. [1970]. These calculations are not very accurate — the upper bound given by the wave function of Fantoni et al. [1970] lies approximately 1.5 MeV above the actual energy for the S3 potential — although the computers at that time were admittedly rather primitive. As mentioned above, it was Tjon [1975] who first attempted solving the Yakubovsky equations directly. His approach leads to an error of several hundred keV in binding energy. Later, hyperspherical harmonic expansions [Ballot, 1981] and Green’s function Monte Carlo methods (GFMC) were used [Zabolitzky et al., 1982], and the accuracy was gradually improved. The ATMS method was the first to give results which are accurate to several tens of keV [Akaishi, 1987]. The IDEA leads to an error of a little less than one MeV. Again, YIE [Kamada and Glöckle, 1992] and YDE [Schellinghout, 1994] agree very well with each other, and also with the ATMS and CHH (hyperspherical) results. Note that the energy calculated using the ATMS method is the expectation value of the
Table 7.4: Convergence of the partial-wave series for the MT-V potential. The subscripts $K$ and $H$ are used as short-hand notations for the $3+1$ and $2+2$ chains, respectively.

<table>
<thead>
<tr>
<th>$\ell_K$</th>
<th>$\ell'_K$</th>
<th>$\ell''_K$</th>
<th>$\ell_H$</th>
<th>$\ell'_H$</th>
<th>$\ell''_H$</th>
<th>$N_c$</th>
<th>YDE</th>
<th>YIE</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1 + 1</td>
<td>$-30.0628(2)$</td>
<td>$-30.07$</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2 + 1</td>
<td>$-30.0587(2)$</td>
<td>$-30.07$</td>
</tr>
<tr>
<td>0</td>
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<td>2</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>3 + 2</td>
<td>$-30.0640(2)$</td>
<td>$-30.07$</td>
</tr>
<tr>
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<td>4</td>
<td>4</td>
<td>0</td>
<td>4</td>
<td>4</td>
<td>5 + 3</td>
<td>$-30.0634(5)$</td>
<td>$-30.07$</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>2 + 2</td>
<td>$-31.0968(2)$</td>
<td>$-31.11$</td>
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<tr>
<td>2</td>
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<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>7 + 5</td>
<td>$-31.1683(5)$</td>
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</tr>
<tr>
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<td>4</td>
<td>3 + 3</td>
<td>$-31.2067(2)$</td>
<td>$-31.20$</td>
</tr>
<tr>
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<td>4</td>
<td>2</td>
<td>4</td>
<td>2</td>
<td>4</td>
<td>13 + 11</td>
<td>$-31.2903(5)$</td>
<td>$-31.3211(5)$</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>24 + 15</td>
<td>$-31.3211(5)$</td>
<td>$-31.3211(5)$</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0</td>
<td>6</td>
<td>0</td>
<td>6</td>
<td>19 + 13</td>
<td>$-31.2188(2)$</td>
<td>$-31.30$</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>2</td>
<td>6</td>
<td>2</td>
<td>6</td>
<td>19 + 13</td>
<td>$-31.3028(5)$</td>
<td>$-31.30$</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
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<td>6</td>
<td>4</td>
<td>6</td>
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<td>$-31.334(4)$</td>
<td>$-31.35$</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>58 + 34</td>
<td>$-31.337(4)$</td>
<td>$-31.36$</td>
</tr>
</tbody>
</table>

Hamiltonian, whereas the YIE and YDE results are Yakubovsky eigenvalues. The experience with the three-body system has shown that this is not a fair comparison. It may be expected that the YIE and YDE variational energies are a significantly tighter upper bound than the ATMS and CHH results.

### 7.5 Possible improvements

Until now, we ({\em i.e.}, Schut and Schellinghout) have not used Cartesian coordinates for the four-body problem. The reason for this is that at the time the four-body project was started, it was not obvious that this could be done efficiently (the three-body problem was at that time also solved using polar coordinates). However, a significant improvement may be expected when Cartesian coordinates are used, for various reasons. Firstly, the operators $Q^\pm$ can be represented in a significantly smaller matrix by changing the Cartesian coordinate pair $(y, z)$ to a polar pair $(\rho, \theta)$. This will lead to a matrix of size and structure similar to that for $P^\pm$. Secondly, the left-hand side may be inverted more cheaply in Cartesian coordinates, since the kinetic energy operator separates more cleanly. Thirdly, the direct potential term can be kept on the left-hand side, to improve the conver-
Table 7.5: Overview of literature values of four-body ground-state energies $E_0$ and comparison with present calculations for the MT-V potential.

<table>
<thead>
<tr>
<th>Method</th>
<th>Ref.</th>
<th>$-E_0$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GFMC</td>
<td>[Zabolitzky et al., 1982]</td>
<td>31.3(2)</td>
</tr>
<tr>
<td>ATMS</td>
<td>[Akaishi, 1987]</td>
<td>31.36</td>
</tr>
<tr>
<td>IDEA</td>
<td>[Oehm et al., 1990]</td>
<td>30.68</td>
</tr>
<tr>
<td>CHH</td>
<td>[Rosati et al., 1992]</td>
<td>31.355</td>
</tr>
</tbody>
</table>

gence. Finally, it is easier to optimize the different grids, since the structure of the Yakubovsky amplitudes is mainly contained in the $\chi$ variable.

A further “improvement” may be achieved by calculating the expectation value of the Hamiltonian instead of the Yakubovsky eigenvalue. This will presumably give more binding energy, and faster convergence, so that less intervals and channels may be used. (The fact that the Yakubovsky eigenvalue has a relative error of approximately $10^{-4}$ suggests that other observables can be calculated with this precision, and the energy with a precision of perhaps $10^{-5}$. This is more than sufficient for most purposes, so that one could do with less intervals and channels.)

7.6 Conclusion

Factorization is even more important in the four-body problem than it is in the three-body problem: standard methods require $O(N^2)$ more storage capacity and $O(N^3)$ more computer time than the methods described in this chapter. However, this can only be achieved by a very careful application of all the methods and tricks that were developed for the three-body problem, and the complexity of the four-body problem makes designing a reliable computer code a highly nontrivial matter. I will discuss some aspects of these problems in Appendix F.

In this chapter, I have shown that the ideas presented in Chapter 5 for the three-body problem can be used for the four-body problem as well. The method has proven to be very successful, and is competitive with any method currently available. Keeping in mind that a relatively small computer was used, and that the method can still be significantly improved, this method appears to be able to become an extremely powerful tool in the four-body problem.