Three-atom scattering via the Faddeev scheme in configuration space.

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Faddeev equations in configuration space and integral form for three-atom scattering processes are formulated allowing for additive and nonadditive forces. The explicit partial wave decomposition is displayed. This formulation appears to be a valuable alternative to current approaches based on hyperspherical harmonic expansion methods of the Schrödinger equation.

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I. INTRODUCTION

The Faddeev scheme for three bodies is a very successful framework in nuclear physics and specifically in the 3-nucleon system [1], [2]. Most of the calculations are performed in momentum space, which is naturally adapted to nuclear forces derived from meson exchange diagrams. Also the coordinate space version of the Faddev equations in differential form has been successfully used, especially for the three-nucleon bound states [3], but an integral equation form of the Faddeev equation in configuration space has not yet been developed in detail. To the best of our knowledge this has not been done before, neither in the fields of nuclear nor atomic physics.

While in nuclear physics there is only one 2-body bound state, the deuteron, diatomic molecules have numerous vibrational and rotational levels. This poses quite a numerical challenge, especially in 3-atom scattering processes. A great deal of work has been done in this field using hyperspherical harmonic expansion methods, [10], [11]. Here and below we quote only a few recent papers. It is the purpose of this paper to describe an alternative approach using the configuration space Faddeev equations in integral form. We have chosen that scheme since over the years a highly efficient numerical technique in coordinate space has been developed by one of us [4] for solving 2-body scattering and bound state problems. This method is based on spectral expansion techniques in terms of Chebyshev polynomials denoted as S-IEM in [4]. As we shall indicate these methods are ideally suited to the integral Faddeev scheme for 3 atoms. It is hoped that this technique will result in an accuracy for the final 3-body results that is higher than what is currently achieved in nuclear physics calculations in momentum space (about 3 significant figures). Needless to say there exist a great demand for theoretical support for various kinds of 3-atom processes: 3-atom recombination processes [12], collisional cooling of co-trapped atomic and molecular ions by ultracold atoms [14], [13], [18], [19], quantum dynamics of ultra cold atom-diatom collisions [15]. Three-atom potential surfaces have been developed, for instance for H3 [16] or for Li3 [17].

In section II we provide a brief derivation of the form of Faddeev equations we want to use. The coordinate space representation expressed in terms of vectors is subsequently set up in section III, while its partial wave representation is worked out in section IV. Because of the complexity of the resulting expressions for general orbital angular momenta a separate section V is devoted to an overall s-wave reduction, since this case provides a more transparent insight into the structure of the equations. Technical details for the partial wave decomposition are deferred to the Appendices. We delegate a numerical feasibility study to a forthcoming paper, but we nevertheless add some remarks on that issue in section VI. Finally in section VII we provide a summary and conclusions.

II. THE THEORETICAL FRAMEWORK

Let us regard a system of three distinguishable atoms, which interact by 2- and 3-atom forces. Though apparently most often the full potential surface for 3 atoms is used ab initio, we prefer to separate out the 2-atom forces from the full potential surface and treat the remainder as a genuine 3-atom force. Thus we denote the total potential energy between 3 atoms by

$$V = V_1 + V_2 + V_3 + V_4$$  \hfill (1)

where the 2-atom forces are conveniently denoted by $V_i \equiv V_{jk}$ (with $j, k \neq i$) and $V_4$ is the genuine 3-atom force. Instead of introducing four Faddeev components corresponding to the four contributions to the potential we split
the 3-atom force into 3 parts, which are then combined with the three 2-atom forces, as follows. We introduce the notation

\[ V_{4} = V_{4}^{(1)} + V_{4}^{(2)} + V_{4}^{(3)} \]  \hspace{1cm} (2)

where \( V_{4}^{(i)} \), \( i = 1, 2, 3 \) has the property of being composed of two pieces, one symmetrical and the other antisymmetrical in the interchange of atoms \( j, k \neq i \). In detail

\[ V_{4} \equiv V(1, 2, 3) = \frac{1}{6}[V(123) + V(132)] + \frac{1}{6}[V(123) - V(132)] \]

\[ + \frac{1}{6}[V(123) + V(321)] + \frac{1}{6}[V(123) - V(321)] \]

\[ + \frac{1}{6}[V(123) + V(213)] + \frac{1}{6}[V(123) - V(213)] \]  \hspace{1cm} (3)

where the argument 123 stands for the space coordinate vectors of the 3 atoms. Thus the two terms in the first row are symmetrical and antisymmetrical, respectively, under exchange of atoms 2 and 3 and similarly for the two terms in next two rows. We group the potential into three terms \( V_{i} \) and \( V_{4}^{(i)} \) in the 3-atom Schrödinger equation (SE), which then can be written as

\[ (H_{0} - E)\Psi = -\sum_{i=1}^{3} (V_{i} + V_{4}^{(i)})\Psi. \]  \hspace{1cm} (4)

In the present paper we describe a scattering process where one atom is incident on a molecular bound state of the other two atoms. We can number the three atoms such that the target molecule is formed out of atoms 2 and 3. Thus the initial channel state is

\[ |\phi_{1} > = |u >_{23} |q_{0} >_{1} \]  \hspace{1cm} (5)

composed of the 2-atom bound state \(|u >\) with quantum numbers to be specified later and a momentum eigenstate \(|q_{0} >_{1}\) of relative motion of atom 1 and the molecule (2,3). That channel state obeys

\[ (H_{0} + V_{1})|\phi_{1} > = E |\phi_{1} > \]  \hspace{1cm} (6)

where \( E \) is the total center of mass energy, and \( H_{0} \) is the kinetic energy operator for the three atoms. The integral form of the SE is

\[ \Psi = G_{0} \left( \sum_{i=1}^{3} (V_{i} + V_{4}^{(i)})\Psi \right) \]  \hspace{1cm} (7)

where where \( G_{0} \) is the free 3-atom propagator, \( G_{0} = (E + i\varepsilon - H_{0})^{-1} \). There is no extra driving term, since there is no solution to the left hand side of Eq.(4) alone which is regular at the origin and purely outgoing. The above equation suggests the decomposition

\[ \Psi \equiv \sum_{i=1}^{3} \psi_{i} \]  \hspace{1cm} (8)

with

\[ \psi_{i} = G_{0}(V_{i} + V_{4}^{(i)})\Psi \]  \hspace{1cm} (9)

Inserting the decomposition \( \Psi \) into the right hand side of Eq.(8) and using the well known identities

\[ (1 - G_{0}V_{1})^{-1}G_{0}V_{1} = G_{0}t_{1} \]

\[ (1 - G_{0}V_{1})^{-1} = 1 + G_{0}t_{1} \]  \hspace{1cm} (10)  \hspace{1cm} (11)

following standard steps \( \S \) \( \S \) one ends up with the 3 coupled Faddeev equations(FE)

\[ \psi_{1} = \phi_{1} + G_{0} t_{1} (\psi_{2} + \psi_{3}) + (1 + G_{0}t_{1})G_{0} V_{4}^{(1)} \Psi \]

\[ \psi_{2} = G_{0} t_{2}(\psi_{3} + \psi_{1}) + (1 + G_{0}t_{2})G_{0} V_{4}^{(2)} \Psi \]

\[ \psi_{3} = G_{0} t_{3}(\psi_{1} + \psi_{2}) + (1 + G_{0}t_{3})G_{0} V_{4}^{(3)} \Psi \]  \hspace{1cm} (12)
The new ingredient, the 2-atom t-operators $t_i$ embedded into the 3-body space, with $i = 1, 2, 3$, obey the Lippmann Schwinger equation (LSE)

$$t_i = V_i + V_i G_0 t_i$$ (13)

This generalization is natural, since the Faddeev equations contain a two-atom potential $V_i$ separately in each arrangement $i$. A short description of the related two-body operator $\tau(r, r')$ and the amplitude $T(r)$ is as follows:

The Lippmann Schwinger equation for the solution of the two-body SE is

$$\psi = \phi + g_0 V \psi,$$

where $g_0$ is the Green’s function $(E_2 + i\epsilon - H_{02})^{-1}$, $H_{02}$ is the two-body kinetic energy operator, $V$ the potential, and $\phi$ is the incident plane wave. The product $V(r) \psi(r)$ is denoted by $T(r)$, and is expressed in terms of an integral involving the $\tau$ operator as

$$V(r) \psi(r) = \int_0^\infty \tau(r, r') \phi(r') \, dr' r'^2.$$ (14)

By manipulating operator identities (10) and (11) one can show that $(1 - V g_0)^{-1} V = \tau$, which is equivalent to Eq. (13), with the difference that $g_0$ contains only the kinetic energy for the relative motion of two particles, while $G_0$ also includes the kinetic energy for the other particle, and further, $E_2$ is the two-body energy, while $E$ is the total three-body energy. The connection between $t_i$ and the two-body $t$-matrix $\tau$ is established in section III, see Eqs (56) and (57).

The kernel pieces in Eqs. (12) determine the asymptotic behavior of the wave function components $\psi_i$ in the outgoing channels. For the 3-atom breakup they can be read off from the expressions standing to the right of the free propagator $G_0$ [1, 8].

Thus if we define the three $T$-amplitudes as

$$\psi_1 = \phi_1 + G_0 \, T_1$$
$$\psi_2 = G_0 \, T_2$$
$$\psi_3 = G_0 \, T_3$$ (15)

then we obtain for the $T_i$ ’s the expressions

$$T_1 = t_1 G_0 (T_2 + T_3) + (1 + t_1 G_0) G_0 \, V_4^{(1)} \Psi$$ (16)

and correspondingly for $T_2$ and $T_3$. The $T$-amplitudes are more useful than the wave function amplitudes because from the $T$-amplitudes one can derive the asymptotic normalization of the wave functions and furthermore, most importantly, the $T$’s decrease to zero at large distances. Inserting Eqs. (15) into the right hand sides of Eq. (16) and the ones for $T_2$ and $T_3$ one finds a set of 3 coupled equations

$$T_1 = t_1 G_0 (T_2 + T_3) + (1 + t_1 G_0) \, V_4^{(1)} \left[ \phi_1 + G_0 \, (T_1 + T_2 + T_3) \right]$$ (17)

$$T_2 = t_2 \phi_1 + (1 + t_2 G_0) \, V_4^{(2)} \left[ \phi_1 + t_2 G_0 (T_3 + T_1) \right]$$
$$+ (1 + t_2 G_0) V_4^{(2)} G_0 (T_1 + T_2 + T_3)$$ (18)

$$T_3 = t_3 \phi_1 + (1 + t_3 G_0) \, V_4^{(3)} \left[ \phi_1 + t_3 G_0 (T_1 + T_2) \right]$$
$$+ (1 + t_3 G_0) V_4^{(3)} G_0 (T_1 + T_2 + T_3)$$ (19)

This is the set of equations which are to be solved. A partial wave decomposition will be given in section IV.

Because of (33), the total breakup amplitude will be

$$U_0 \equiv T_1 + T_2 + T_3$$ (20)

from which the physical breakup amplitude can be obtained by calculating the matrix element

$$< \phi_0 | U_0 >$$ (21)

where $| \phi_0 >$ is a product of momentum eigenstates for the free motion of the three atoms in the final state.

One is also interested in the transition amplitudes for elastic and rearrangement scattering. They can be read off from Eqs. (12) by rewriting the kernel parts such that $V_i$ distorts the Green operators

$$G_i = \frac{1}{E + i\epsilon - H_0 - V_i}$$ (22)
Since $G_0 t_i = G_i V_i$, with $(1 + G_0 t_i)G_0 = G_i$, one finds for the elastic transition amplitude

$$U_{11} = V_1(\psi_2 + \psi_3) + V_4^{(1)}\Psi$$

and for the two rearrangement amplitudes

$$U_{21} = V_2(\psi_3 + \psi_1) + V_4^{(2)}\Psi$$
$$U_{31} = V_3(\psi_1 + \psi_2) + V_4^{(3)}\Psi$$

Upon inserting (15) into the above expressions for the $U$’s, we obtain

$$U_{11} = V_1 G_0 (T_2 + T_3) + V_4^{(1)}[\phi_1 + G_0(T_1 + T_2 + T_3)]$$

$$U_{21} = V_2[\phi_1 + G_0(T_3 + T_1)] + V_4^{(2)}[\phi_1 + G_0(T_1 + T_2 + T_3)]$$
$$U_{31} = V_3[\phi_1 + G_0(T_1 + T_2)] + V_4^{(3)}[\phi_1 + G_0(T_1 + T_2 + T_3)]$$

The physical amplitudes are

$$<\phi_i|U_{11}>$$

where the $\phi_i$’s obey the SE

$$V_i|\phi_i> = (E - H_0)|\phi_i>$$

Like in Eq. (14) the channel states $\phi_2$ and $\phi_3$ contain bound states. Thus when calculating the matrix elements (29), one can replace $V_i\phi_i$ by $G_0^{-1}\phi_i$, and hence replace $V_i G_0$ in Eqs. (26), (27), (28) by 1. These substitutions then lead to the final expressions

$$U_{11} = (T_2 + T_3) + V_4^{(1)}[\phi_1 + G_0 (T_1 + T_2 + T_3)]$$
$$U_{21} = G_0^{-1}\phi_1 + (T_3 + T_1) + V_4^{(2)}[\phi_1 + G_0 (T_1 + T_2 + T_3)]$$
$$U_{31} = G_0^{-1}\phi_1 + (T_1 + T_2) + V_4^{(3)}[\phi_1 + G_0 (T_1 + T_2 + T_3)]$$

It can easily be verified that the forms in the equations above for the $U_{11}$ are identical to the more standard expressions, which are

$$U_{11} = (V_j + V_k + V_4)\Psi, \quad j, k \neq i$$

For instance one has

$$<\phi_1|U_{11}> = <\phi_1|V_1(\psi_2 + \psi_3)> + <\phi_1|V_4^{(1)}|\Psi>$$
$$= <\phi_1|G_0^{-1}(\psi_2 + \psi_3)> + <\phi_1|V_4^{(1)}|\Psi>$$
$$= <\phi_1|G_0^{-1}|\Psi> - <\phi_1|G_0^{-1}\psi_1> + <\phi_1|V_4^{(1)}|\Psi>$$
$$= <\phi_1|V_1 + V_2 + V_3 + V_4|\Psi> - <\phi_1|G_0^{-1}G_0(V_1 + V_4^{(1)})|\Psi>$$
$$+ <\phi_1|V_4^{(1)}|\Psi>$$
$$= <\phi_1|V_2 + V_3 + V_4^{(1)}|\Psi>$$

In the second to last step we used the definition of the Faddeev amplitudes, Eq. (14).

In the case of identical atoms the 3 Faddeev amplitudes (11) are identical in form, only the particles are permuted. One easily finds

$$\psi_2 + \psi_3 = \mathcal{P}\psi_1$$

(36)
where
\[ \mathcal{P} = P_{12}P_{23} + P_{13}P_{21} \]  
(37)
is a sum of a cyclical and anticyclical permutations of 3 objects. Thus the total state can be written as
\[ \Psi = (1 + \mathcal{P})\psi_1 \]  
(38)
and hence only one FE is needed that reads
\[ \psi_1 = \phi_1 + G_0 t_1 \mathcal{P} \psi_1 + (1 + G_0 t_1)G_0 V_4^{(1)}(1 + \mathcal{P})\psi_1 \]  
(39)
? If one defines again
\[ \psi_1 = \phi_1 + G_0 T \]  
(40)
then the amplitude \( T \) obeys
\[ T = t_1 \mathcal{P} \phi_1 + (1 + t_1 G_0)V_4^{(1)}(1 + \mathcal{P})\phi_1 
+ t_1 \mathcal{P} G_0 T + (1 + t_1 G_0)V_4^{(1)}(1 + \mathcal{P})G_0 T \]  
(41)
The driving term in (41) is contained in the first line and the integral operator is contained in the second line. The complete break up amplitude is
\[ U_0 = (1 + \mathcal{P})T \]  
(42)
Because of the identity of the atoms there is only one amplitude for the transition into two-body fragmentation, which, according to Eq. (39) is
\[ U = V_1 \mathcal{P} \psi_1 + V_4^{(1)}(1 + \mathcal{P})\psi_1 
= \mathcal{P}G_0^{-1}\phi_1 + \mathcal{P}T + V_4^{(1)}(1 + \mathcal{P})\phi_1 + V_4^{(1)}(1 + \mathcal{P})G_0 T \]  
(43)
The last expression is valid for calculating the physical matrix element \( <\phi_1|U> \).
This concludes the derivation of the formal framework. The case where only two atoms are identical is similar to the above and is left to the reader.

III. COORDINATE SPACE REPRESENTATION

In a 3-atom system there are three 2-body fragmentation ( or arrangement ) channels going with three types of Jacobi vectors ( \( ijk = 123 \) and cyclical permutations)
\[ \bar{x}^{(i)} = \bar{x}_j - \bar{x}_k; \quad \bar{y}^{(i)} = \bar{x}_i - \frac{m_j}{m_j + m_k} \bar{x}_j - \frac{m_k}{m_j + m_k} \bar{x}_k \]  
(44)
We introduce coordinate space states
\[ |\bar{x} \bar{y}>_1 \equiv |\bar{x}^{(1)}, \bar{y}^{(1)}> \]  
(45)
\[ |\bar{x} \bar{y}>_2 \equiv |\bar{x}^{(2)}, \bar{y}^{(2)}> \]  
(46)
\[ |\bar{x} \bar{y}>_3 \equiv |\bar{x}^{(3)}, \bar{y}^{(3)}> \]  
(47)
Each set of states is complete:
\[ \int d\bar{x}d\bar{y} |\bar{x} \bar{y}> <\bar{x} \bar{y}| = 1. \]  
(48)
The various terms for the \( T \)-amplitudes in Eqs. (17) - (19) will now be written in the coordinate space representation, using the definitions in Eqs. (45) - (47). It is natural to represent the amplitude \( T_1 \) as \( _1 <\bar{x} \bar{y}|T_1> \), \( T_2 \) as
where each is diagonal in momentum space. We use Jacobi momenta $\mu$ and $M_i$ and $M_j$ in equation (13), which in configuration space reads

$$<\vec{x}\vec{y}> = <\vec{x}\vec{y}|V|\vec{x}'\vec{y}'> \int d\vec{x}'d\vec{y}' <\vec{x}'\vec{y}'|G_0|\vec{x}''\vec{y}'' > + 1 <\vec{x}''\vec{y}''|G_0|\vec{x}''\vec{y}'' >$$

Various matrix elements occur which we now consider one by one. The 2-body $t$-matrix obeys the Lippmann Schwinger equation (13), which in configuration space reads

$$<\vec{x}\vec{y}|V|\vec{x}'\vec{y}'> = \delta(\vec{y} - \vec{y}') <\vec{x}|V|\vec{x}'> = \frac{1}{(2\pi)^3} \int d\vec{q} e^{i\vec{q}\cdot(\vec{y} - \vec{y}') <\vec{x}|V|\vec{x}'>}$$

The three-body free Green’s function can be related to a two-body free Green’s function, by making use of the property that each is diagonal in momentum space. We use Jacobi momenta $\vec{p}(i)$, $\vec{q}(i)$ related to $\vec{x}(i)$, $\vec{y}(i)$ and obtain

$$<\vec{x}\vec{y}|G_0|\vec{x}'\vec{y}'> = \int d\vec{p} d\vec{q} <\vec{x}\vec{y}|\vec{p}\vec{q} > \frac{1}{E + \frac{q^2}{2M_0} - \frac{q^2}{2M_i}} <\vec{p}\vec{q}|\vec{x}'\vec{y}'>$$

$$\equiv \frac{1}{(2\pi)^3} \int d\vec{q} e^{i\vec{q}\cdot(\vec{y} - \vec{y}') g(\vec{x}, \vec{x}'; \epsilon_q)}$$

where $g(\vec{x}, \vec{x}'; \epsilon_q)$ is the well known free single particle Greens function

$$g(\vec{x}, \vec{x}'; \epsilon_q) = \frac{i\epsilon_q}{2\pi} e^{-\sqrt{2\mu_1(\epsilon_q - E - i\eta)}} |\vec{x} - \vec{x}'|$$

We introduced the reduced mass $\mu_i$ of the two atoms in the arrangement (i)

$$\mu_i = \frac{m_j m_k}{m_j + m_k}$$

and $M_i$ the reduced mass between the particle i and the pair ( jk)

$$M_i = \frac{m_i (m_j + m_k)}{m_i + m_j + m_k}$$

and $\epsilon_q \equiv E - \frac{\vec{q}^2}{2M_i}$ is the energy related to the 2- atom subsystem.

Similarly, we can relate the two-body $t$-matrix embedded in the three-body space to the two-body $\tau$-matrix defined in the two-body space as follows. Inserting (51) and (52) into the LSE (49) it follows that the $t$-matrix has the form

$$<\vec{x}\vec{y}|t|\vec{x}'\vec{y}'> = \frac{1}{(2\pi)^3} \int d\vec{q} e^{i\vec{q}\cdot(\vec{y} - \vec{y}') <\vec{x}|\tau(\epsilon_q)|\vec{x}'>}$$

where $\tau(\vec{x}, \vec{x}'\epsilon_q) \equiv <\vec{x}|\tau(\epsilon_q)|\vec{x}'>$ obeys the two-body LSE

$$\tau(\vec{x}, \vec{x}'; \epsilon_q) = V(x)\delta(\vec{x} - \vec{x}') + \int d\vec{x}'' V(x)g(\vec{x}, \vec{x}''; \epsilon_q)\tau(\vec{x}'', \vec{x}'; \epsilon_q),$$
Therefore, together with (72), (56), (52) we obtain

\[
\begin{align*}
\vec{x}^{(2)} &= A\vec{x}^{(1)} + B\vec{y}^{(1)} \\
\vec{y}^{(2)} &= C\vec{x}^{(1)} + D\vec{y}^{(1)}
\end{align*}
\]

Similarly

\[
\begin{align*}
\vec{x}^{(3)} &= A'\vec{x}^{(1)} + B'\vec{y}^{(1)} \\
\vec{y}^{(3)} &= C'\vec{x}^{(1)} + D'\vec{y}^{(1)}
\end{align*}
\]

where

\[
\begin{align*}
A &= -\frac{m_2}{m_2 + m_3} && B = -1 \\
C &= \frac{m_3}{m_2 + m_3} \frac{m_1 + m_2 + m_3}{m_1 + m_3} && D = -\frac{m_1}{m_1 + m_3} \\
A' &= -\frac{m_3}{m_2 + m_3} && B' = 1 \\
C' &= -\frac{m_2}{m_2 + m_3} \frac{m_1 + m_2 + m_3}{m_1 + m_2} && D' = -\frac{m_1}{m_1 + m_2}
\end{align*}
\]

As a consequence one can express the state \(|\vec{x} \vec{y}>_1\) as

\[
\begin{align*}
|\vec{x} \vec{y}>_1 &= |A\vec{x} + B\vec{y}, C\vec{x} + D\vec{y}>_2 \\
|\vec{x} \vec{y}>_1 &= |A'\vec{x} + B'\vec{y}, C'\vec{x} + D'\vec{y}>_3 \\
&= |A'\vec{x} + B'\vec{y}, C'\vec{x} + D'\vec{y}> + |A\vec{x} + B\vec{y}, C\vec{x} + D\vec{y}> >_2
\end{align*}
\]

The above equations mean that a spatial configuration represented in arrangement 1 by vectors \(\vec{x}\) and \(\vec{y}\) is represented in arrangement 2 by vectors \(A\vec{x} + B\vec{y}\) and \(C\vec{x} + D\vec{y}\) and similarly for arrangement 3. This leads to

\[
\begin{align*}
1 < \vec{x} \vec{y}|T_2 + T_3 &> = \frac{1}{(2\pi)^7} \int d\vec{x}'' \int d\vec{y}'' \int d\vec{x}'' \\
& \times e^{i\vec{x}(\vec{x}' - \vec{x}'')} \langle \vec{x} \vec{y}|V_4^{(1)}|\vec{x} \vec{y}>_1 < \vec{x} \vec{y}|\phi_1 > \\
& + \int d\vec{x}'' d\vec{y}' < \vec{x} \vec{y}|t_1 G_0||\vec{x} \vec{y}>_1 \int d\vec{x}''' d\vec{y}'' |V_4^{(1)}|\vec{x}''' \vec{y}''>_1 < \vec{x}''' \vec{y}''|\phi_1 >
\end{align*}
\]

Thus the unknown amplitudes \(2 < \vec{x} \vec{y}|T_2 >\) and \(3 < \vec{x} \vec{y}|T_3 >\) occur with shifted arguments under the integral.

Next we regard the second term on the right hand side of Eq. (64):

\[
\begin{align*}
1 < \vec{x} \vec{y}|(1 + t_1 G_0)V_4^{(1)}|\phi_1 > &= \int d\vec{x}'' d\vec{y}' < \vec{x} \vec{y}|V_4^{(1)}|\vec{x} \vec{y} >_1 < \vec{x} \vec{y}|\phi_1 > \\
& + \int d\vec{x}'' d\vec{y}' < \vec{x} \vec{y}|t_1 G_0||\vec{x} \vec{y}>_1 \int d\vec{x}''' d\vec{y}'' |V_4^{(1)}|\vec{x}''' \vec{y}''>_1 < \vec{x}''' \vec{y}''|\phi_1 >
\end{align*}
\]

The 3- atom force \(V_4^{(1)}\) has to be a scalar under rotations. Therefore for spinless atoms and assuming locality it will have the form

\[
1 < \vec{x} \vec{y}|V_4^{(1)}|\vec{x} \vec{y} >_1 = V^{(1)}(x, y, \vec{x} \cdot \vec{y})\delta(\vec{x} - \vec{x}')\delta(\vec{y} - \vec{y}')
\]

Therefore, together with (72), (56), (62) we obtain

\[
\begin{align*}
< \vec{x} \vec{y}|(1 + t_1 G_0)V_4^{(1)}|\phi_1 > &= V^{(1)}(x, y, \vec{x} \cdot \vec{y})u(x)\frac{1}{(2\pi)^3/2}e^{i\vec{x} \cdot \vec{y}} \\
& + \frac{1}{(2\pi)^7} \int d\vec{y}'' \int d\vec{x}'' \int d\vec{y}'\tau(\vec{x}, \vec{x}'', \vec{y}'') \int d\vec{x}'' \tau(\vec{x}, \vec{x}'', \vec{y}'') \\
& \cdot g(\vec{x}'', \vec{x}''; \epsilon_q) V^{(1)}(x', y', \vec{x}' \cdot \vec{y}') u(x')\frac{1}{(2\pi)^3/2}e^{i\vec{x}' \cdot \vec{y}'}
\end{align*}
\]
Finally the third term on the right hand side of Eq. (17) can be transformed by means of similar steps with the result

\[ <\vec{x} \vec{y}^r(1 + t_1 G_0) \]

\[ V_4^{(1)} G_0(T_1 + T_2 + T_3) > \tag{74} \]

\[ = V^{(1)}(x, y, \hat{\vec{y}}) \frac{1}{(2\pi)^3} \int dq \int dx \int dh \bar{e}^{i\vec{q} \cdot (\vec{y} - \vec{y}')} g(\vec{x}, \vec{y}'; \epsilon_q) \]

\[ (<\vec{x} \vec{y}^r | T_1 > + < A\vec{x}^r + B\vec{y}^r, C\vec{x}, D\vec{y}^r | T_2 > + < A'\vec{x}^r + B'\vec{y}^r, C'\vec{x}, D'\vec{y}^r | T_3 > ) \]

\[ + \frac{1}{(2\pi)^3} \int dq \int dq' e^{i\vec{q} \cdot (\vec{y} - \vec{y}')} \int dx \int dx' \tau(\vec{x}, \vec{x}'; \epsilon_q) g(\vec{x}, \vec{x}'; \epsilon_q) \]

\[ V^{(1)}(x', y', \hat{\vec{x}}'; \hat{\vec{y}}') \frac{1}{(2\pi)^3} \int dq \int dx' \int dh' \bar{e}^{i\vec{q}' \cdot (\vec{y}' - \vec{y}')} g(\vec{x}', \vec{y}'', \epsilon_q) \]

\[ (<\vec{x}' \vec{y}'^r | T_1 > + < A\vec{x}'^r + B\vec{y}'^r, C\vec{x}'^r, D\vec{y}'^r | T_2 > + < A'\vec{x}'^r + B'\vec{y}'^r, C'\vec{x}', D'\vec{y}'^r | T_3 > ) \]

We leave it to the reader to work out the coordinate space representations for the remaining two equations (18), (19).

In case of identical particles there is only one FE given by (11) to be solved for the amplitude \( T(\vec{x}, \vec{y}) \equiv <\vec{x} \vec{y}|T > \). This equation is of the form

\[ T = T^0 + K \tag{75} \]

where \( T^0 \) is the driving term and \( K \) incorporates the \( T \)- amplitudes. In the coordinate space representation

\[ T^0(\vec{x}, \vec{y}) = \frac{4}{3} \frac{1}{\pi^{3/2}} \int dq \int dq' \int dh \bar{e}^{i\vec{q} \cdot (\vec{y} - \vec{y}')} \]

\[ [\tau(\vec{x}, \vec{y}'; \epsilon_q) u_{\vec{x}}(\vec{x}, \vec{y}'; \epsilon_q) u_{\vec{y}}(\vec{x}, \vec{y}'; \epsilon_q) e^{i\vec{q} \cdot \vec{y}'} \]

\[ + V^{(1)}(x, y, \hat{\vec{x}} \cdot \hat{\vec{y}}) \frac{1}{(2\pi)^3} [u_{\vec{x}}(\vec{x}, \vec{y}; \epsilon_q) e^{i\vec{q} \cdot \vec{y}} \]

\[ + u_{\vec{x}}(\vec{x}, \vec{y}; \epsilon_q) e^{i\vec{q} \cdot (\vec{x} - \vec{y})} + u_{\vec{x}}(-\frac{1}{2} \vec{x} - \vec{y}) e^{i\vec{q} \cdot (\vec{x} - \vec{y})} \]

\[ + \frac{1}{(2\pi)^3} \int dq \int dq' \int dx' \int dx'' e^{i\vec{q} \cdot (\vec{y} - \vec{y}'')} \int dx \int dx' \tau(\vec{x}, \vec{x}'; \epsilon_q) g(\vec{x}, \vec{x}'; \epsilon_q) \]

\[ V^{(1)}(x', y', \hat{\vec{x}}', \hat{\vec{y}}') \frac{1}{(2\pi)^3} [(u_{\vec{x}}(\vec{x}'; \epsilon_q) e^{i\vec{q} \cdot \vec{y}} \]

\[ + u_{\vec{x}}(\vec{x}'; \epsilon_q) e^{i\vec{q} \cdot (\vec{x}' - \vec{y}')} + u_{\vec{x}}(-\frac{1}{2} \vec{x}' - \vec{y}') e^{i\vec{q} \cdot (\vec{x}' - \vec{y}')}} \]

and

\[ K(\vec{x} \vec{y}) = \frac{1}{(2\pi)^3} \int dx \int dx' \int dh \bar{e}^{i\vec{q} \cdot (\vec{y} - \vec{y}'')} \int dx \int dx' \tau(\vec{x}, \vec{x}'; \epsilon_q) g(\vec{x}, \vec{x}'; \epsilon_q) \]

\[ [T(-\frac{1}{2} \vec{x}' - \vec{y}'; \epsilon_q) \frac{1}{2} \vec{x}' - \frac{1}{4} \vec{x}' - \frac{1}{2} \vec{y}'') + T(-\frac{1}{2} \vec{x}' + \vec{y}'; \epsilon_q) \]

\[ + V^{(1)}(x, y, \hat{\vec{x}} \cdot \hat{\vec{y}}) \frac{1}{(2\pi)^3} \int dq \int dq' \int dx' \int dx'' g(\vec{x}, \vec{x}''; \epsilon_q) \]

\[ + < A\vec{x} + B\vec{y}, C\vec{x} + D\vec{y} | T + < A'\vec{x} + B'\vec{y}, C'\vec{x} + D'\vec{y} | T > \]

\[ + \frac{1}{(2\pi)^3} \int dq \int dq' \int dx' \int dx'' e^{i\vec{q} \cdot (\vec{y} - \vec{y}'')} \int dx \int dx' \tau(\vec{x}, \vec{x}'; \epsilon_q) g(\vec{x}', \vec{x}''; \epsilon_q V^{(1)}(x', y', \hat{\vec{x}} \cdot \hat{\vec{y}}) \]

\[ + \frac{1}{(2\pi)^3} \int dq \int dq' e^{i\vec{q} \cdot (\vec{y} - \vec{y}'')} g(\vec{x}, \vec{x}''; \epsilon_q) \]

\[ [<\vec{x}' \vec{y}'^r] T > + < A\vec{x}' + B\vec{y}'^r, C\vec{x}'^r + D\vec{y}'^r | T > \]

\[ + < A'\vec{x}' + B'\vec{y}'^r, C'\vec{x}'^r + D'\vec{y}'^r | T > \]
Once the amplitude $T(\vec{x}, \vec{y})$ has been determined the physical 3– atom break up matrix element is obtained as

$$< \vec{p} \vec{q} | U_0 > \equiv < \vec{p} \vec{q} | (1 + P)T > = \frac{1}{(2\pi)^3} \int d\vec{x} \, d\vec{y} \, e^{-i\vec{p} \cdot \vec{x}} e^{-i\vec{q} \cdot \vec{y}} \, T(\vec{x}, \vec{y}) + \text{permuted parts}$$

The permuted parts are most conveniently evaluated by applying the permutation $P$ to the left:

$$1 < \vec{p} \vec{q} | P = 2 < \vec{p} \vec{q} | + 3 < \vec{p} \vec{q} |$$

Then one expresses the Jacobi momenta of the type 1 in terms of the Jacobi momenta of the types 2 and 3. One has

$$\vec{p}^{(1)} = -\frac{1}{2} \vec{p}^{(2)} + \frac{3}{4} \vec{q}^{(2)}$$

$$\vec{q}^{(1)} = -\vec{p}^{(2)} - \frac{1}{2} \vec{q}^{(2)}$$

$$\vec{p}^{(1)} = -\frac{1}{2} \vec{p}^{(3)} - \frac{3}{4} \vec{q}^{(3)}$$

$$\vec{q}^{(1)} = \vec{p}^{(3)} - \frac{1}{2} \vec{q}^{(3)}$$

and therefore

$$2 < \vec{p} \vec{q} | = 1 < -\frac{1}{2} \vec{p}^{(2)} + \frac{3}{4} \vec{q}^{(2)} - \vec{p} + \frac{1}{2} \vec{q}^{(2)}$$

and similarly for 3 < \vec{p} \vec{q} | . Thus altogether

$$< \vec{p} \vec{q} | U_0 > = T(\vec{p} \vec{q}) + T(-\frac{1}{2} \vec{p} + \frac{3}{4} \vec{q} - \vec{p} - \frac{1}{2} \vec{q}) + T(-\frac{1}{2} \vec{p} - \frac{3}{4} \vec{q}, \vec{p} - \frac{1}{2} \vec{q})$$

It remains to display the physical matrix element $< \phi'_1 | U >$ for elastic and inelastic scattering , where $| \phi'_1 > = | u' > | \vec{q} >$ represents the final state. According to \[8\] one obtains

$$< \phi'_1 | U > = < \phi'_1 | PG_{0}^{-1} | \phi_1 > + < \phi'_1 | P | T > + < \phi'_1 | V^{(1)}(1 + P)G_0 T >$$

For the first term we can use the SE for $\phi_1$ and obtain

$$< \phi'_1 | PG_{0}^{-1} | \phi_1 > = < \phi'_1 | PV | \phi_1 > = \int d\vec{x}' \, d\vec{y}' \, d\vec{x}'' \, d\vec{y}'' \, < \phi'_1 | \vec{x}' \vec{y}' >_1 \, < \vec{x}' \vec{y}' | P | \vec{x}'' \vec{y}'' >_1 \, < \vec{x}'' \vec{y}'' | V | \phi_1 >$$

This is an example where one might evaluate the $P$ -matrix element differently from the one shown above. The expressions \[68\], \[69\] can be rewritten as

$$1 < \vec{x} \vec{y} | P | \vec{x}' \vec{y}' >_1 = (\frac{1}{C})^3 \delta(\vec{x} - \frac{1}{C} \vec{y}) - \frac{D}{C} \frac{D'}{C'} \delta(\vec{x} - \frac{A}{C} \vec{y}' - \frac{AD - BC}{C} \vec{y})$$

$$+ (\frac{1}{C'})^3 \delta(\vec{x} - \frac{1}{C'} \vec{y}' - \frac{D'}{C'} \vec{y}) \delta(\vec{x}' - \frac{A'}{C} \vec{y}' - \frac{A'D' - B'C'}{C} \vec{y})$$

For identical atoms one has $A = -\frac{1}{2}, B = -1, C = \frac{1}{2}, D = -\frac{1}{2}, A' = -\frac{1}{2}, B' = 1, C' = -\frac{1}{2}, D' = -\frac{1}{2}$. Then we obtain

$$< \phi'_1 | PG_{0}^{-1} | \phi_1 > = < \phi'_1 | PV | \phi_1 > = \frac{1}{(2\pi)^3} (\frac{4}{3})^3 \int d\vec{y}' \int d\vec{y}'' e^{-i\vec{q} \cdot \vec{y}' + i\vec{q} \cdot \vec{y}''}$$

$$\left( u_{n}^{*}(\frac{4}{3} \vec{y}' + \frac{2}{3} \vec{y}) V(\frac{2}{3} \vec{y}' + \frac{4}{3} \vec{y}) u_{n}(\frac{2}{3} \vec{y}' - \frac{4}{3} \vec{y}) + u_{n}^{*}(\frac{-4}{3} \vec{y}' - \frac{2}{3} \vec{y}) V(\frac{2}{3} \vec{y}' + \frac{4}{3} \vec{y}) u_{n}(\frac{2}{3} \vec{y}' + \frac{4}{3} \vec{y}) \right)$$
This together with the remaining terms on the right hand side of (87) yields
\[ < \phi_1 | U > = \frac{1}{(2\pi)^3} \int d\vec{y} \int d\vec{y'} e^{-i\vec{q} \cdot \vec{y}} e^{i\vec{q'} \cdot \vec{y'}} \]
\[ [u_n^*(\frac{4}{3} \vec{y} + \frac{2}{3} \vec{y'}) V((\frac{2}{3} \vec{y} + \frac{4}{3} \vec{y'})) u_m(\frac{4}{3} \vec{y} - \frac{4}{3} \vec{y'}) + u_n^*(\frac{4}{3} \vec{y} - \frac{4}{3} \vec{y'}) V((\frac{2}{3} \vec{y} + \frac{4}{3} \vec{y'})) u_m(\frac{4}{3} \vec{y} + \frac{4}{3} \vec{y'})] \]
\[ + \frac{1}{(2\pi)^{3/2}} \int d\vec{y} \int d\vec{y'} e^{-i\vec{q} \cdot \vec{y}} u_n^*(\frac{4}{3} \vec{y} + \frac{2}{3} \vec{y'}) T(\frac{2}{3} \vec{y} - \frac{4}{3} \vec{y'}) + u_n^*(\frac{4}{3} \vec{y} - \frac{4}{3} \vec{y'}) T(\frac{2}{3} \vec{y} + \frac{4}{3} \vec{y'}) \]
\[ + \frac{1}{(2\pi)^{3/2}} e^{-i\vec{q} \cdot \vec{y}} u_n^*(\vec{x}) V(1)(xy, \hat{x} \cdot \vec{y}) [u_n(\vec{x}) e^{i\vec{q} \cdot \vec{y}} + u_m(-\frac{1}{2} \vec{x} - \vec{y}) e^{i\vec{q} \cdot \vec{y}}] \]
\[ + \frac{1}{(2\pi)^{3/2}} e^{-i\vec{q} \cdot \vec{y}} u_n^*(\vec{x}) V(1)(xy, \hat{x} \cdot \vec{y}) \int d\vec{y} \int d\vec{y'} \int d\vec{x} e^{i\vec{q} \cdot \vec{y}} g(\vec{x}, \vec{x'}; \epsilon_q) \]
\[ < \vec{x}' \vec{y}'| T > + < A\vec{x}' + B\vec{y}', C\vec{x} + D\vec{y}' | T > + < A\vec{x}' + B\vec{y}', C\vec{x} + D\vec{y}' | T > \]

For distinguishable particles corresponding results occur and their evaluation is left to the reader.

IV. PARTIAL WAVE DECOMPOSITION

In view of the various vibration-rotational levels it is natural to decompose the integral equations for the various T-amplitudes into partial waves. We exemplify that step for the case of three identical atoms, and choose therefore Eqs. 75, 76, 77. The scalar quantities \( T \) as well as the single particle Green’s function \( g \), both contained in Eqs. 75, 76, 77, have the partial wave decomposition

\[ \tau(\vec{x}, \vec{x'}; \epsilon_q) = \sum_{l,m} Y_{l,m}(\hat{x}) \tau_l(x, x'; \epsilon_q) Y_{l,m}^*(\hat{x'}) \]
(93)

\[ g(\vec{x}, \vec{x'}; \epsilon_q) = \sum_{l,m} Y_{l,m}(\hat{x}) g_l(x, x'; \epsilon_q) Y_{l,m}^*(\hat{x'}) \]
(94)

and

\[ \delta(\vec{x} - \vec{x'}) = \sum_{l,m} Y_{l,m}(\hat{x}) Y_{l,m}^*(\hat{x'}) \]
(95)

Here \( \hat{v} \) is the unit vector pointing in the direction of \( \vec{v} \). When used as an argument of a spherical harmonics \( \hat{v} \) stands for the angles \( \theta \) and \( \phi \).

As a consequence the LSE for \( \tau \), Eq. 57, for a given angular momentum \( l \) reads

\[ \tau_l(x, x'; \epsilon_q) = V(x) \frac{\delta(x - x')}{xx'} \]
\[ + V(x) \int_0^{\infty} dx'' x'' g(x, x''; \epsilon_q) \tau_l(x'', x'; \epsilon_q) \]
(96)

Further ingredients are the initial bound state

\[ u_{n_0}(\vec{x}) = u_{n_0}(x) Y_{l_0,m_0}(\hat{x}) \]
(97)

and the standard expansion of the plane wave

\[ e^{i \vec{q} \cdot \vec{y}} = 4\pi \sum_{\lambda, \mu} i^\lambda j_\lambda(qy) Y_{\lambda, \mu}^*(\hat{y}) Y_{\lambda, \mu}((\hat{y}) \]
(98)

Next one introduces bi-polar spherical harmonics of total angular momentum \( L \)

\[ Y_{l_1, l_2}^{L,M}(\hat{x}, \hat{y}) \equiv \sum_{m_1, m_2} C(l_1l_2, m_1m_2) Y_{l_1,m_1}(\hat{x}) Y_{l_2,m_2}(\hat{y}) \]
(99)
where the \( C(\cdots) \) is a Clebsch-Gordan coefficients as defined in \( \text{[5]} \). However, in what follows we are going to omit the third magnetic quantum number, since \( m + \mu = M \).

Using the notation above we will now begin to evaluate the amplitude \( T \) given in Eqs. \( \text{[1]} \) and \( \text{[2]} \) of \( \text{[11]} \). The two driving terms in the first line of Eq. \( \text{[11]} \) will be denoted by \( T^{0,1} \) and \( T^{0,2} \), respectively.

As an intermediate result one obtains for \( T^{0,1} \)

\[
\langle \vec{x} \vec{y}|T^{0,1}\rangle = \frac{4}{3} \frac{1}{(2\pi)^{3/2}} (4\pi)^3 \sum_{LM} \sum_{\lambda\lambda'} Y^{L,M}_{\lambda\lambda'}(\hat{x}, \hat{y})
\]

\[
\times \int_0^\infty dq q^2 j_\lambda(qy) \int_0^\infty dy' dy'^2 j_\lambda(qy') Y^{L,M}_{\lambda\lambda'}(\frac{4}{3} \hat{y}' + \frac{2}{3} \hat{y}, \hat{y}')
\]

\[
\times \tau(x, |\frac{4}{3} \hat{y}' + \frac{2}{3} \hat{y}|; \varepsilon_q) u_{n_0}(\frac{2}{3} \hat{y}' + \frac{4}{3} \hat{y}') \sum_{\lambda_0\mu_0} i^{\lambda_0} j_{\lambda_0}(qy'') Y^{L,M}_{\lambda_0,\mu_0}(\hat{q}_0)
\]

\[
\sum_{L'} C(l_0\lambda_0 L', m_0, \mu_0) Y^{L',m_0+\mu_0}_{l_0,\lambda_0}(\frac{2}{3} \hat{y}' + \frac{4}{3} \hat{y}', \hat{y}'') [(-)^{l_0} + (-)^{l'}],
\]

where \( t \) is the cosine of the angle between the vectors \( \vec{y}' \) and \( \vec{y} \). After placing \( \hat{q}_0 \) into the \( \hat{z} \) direction we obtain

\[
\langle \vec{x} \vec{y}|tP|\phi \rangle = \frac{4}{3} \frac{1}{(2\pi)^{3/2}} (4\pi)^3 \sum_{LM} \sum_{\lambda\lambda'} Y^{L,M}_{\lambda\lambda'}(\hat{x}, \hat{y})
\]

\[
\times \int_0^\infty dq q^2 j_\lambda(qy) \int_0^\infty dy' dy'^2 j_\lambda(qy') Y^{L,M}_{\lambda\lambda'}(\frac{4}{3} \hat{y}' + \frac{2}{3} \hat{y}, \hat{y}')
\]

\[
\times \int d\hat{y}' \int d\hat{y}'' Y^{L,M}_{\lambda\lambda'}(\frac{4}{3} \hat{y}' + \frac{2}{3} \hat{y}, \hat{y}') \sum_k (2\pi)\sqrt{2k} + 1(-)^k Y^{L,M}_{\lambda_0,\lambda_0}(\hat{q}_0, \hat{y}'') G_k
\]

\[
\sum_{\lambda_0} j_{\lambda_0}(qy'') \sqrt{(2\lambda_0 + 1)/(4\pi)}
\]

\[
\sum_{L'} C(l_0\lambda_0 L', m_0, 0) Y^{L',m_0}_{l_0,\lambda_0}(\frac{2}{3} \hat{y}' + \frac{4}{3} \hat{y}', \hat{y}'') [(-)^{l_0} + (-)^{l'}].
\]

The remaining angular integrations can be performed analytically with the result

\[
\int d\hat{y}' \int d\hat{y}'' Y^{L,M}_{\lambda\lambda'}(\frac{4}{3} \hat{y}' + \frac{2}{3} \hat{y}, \hat{y}') Y^{L,M}_{\lambda_0,\lambda_0}(\frac{2}{3} \hat{y}' + \frac{4}{3} \hat{y}, \hat{y}'') = \delta_{L,L'} \delta_{M,m_0} h^{L,M}_{\lambda_0,\lambda_0}(\hat{y}', \hat{y}'')
\]

where the explicit expression for \( h \) is given in Appendix A.

The \( t \)-matrix occurring in Eq. \( \text{[11]} \) contains as a driving term the function \( V(x) \delta(x-x')/x x' \) (see Eq. \( \text{[1]} \)). It is more convenient to explicitly separate this term out by defining the function \( r_t \)

\[
\tau_t(x, x'; \varepsilon_q) = V(x) \frac{\delta(x-x')}{xx'} + r_t(x, x'; \varepsilon_q)
\]
and treat the $\delta$-function term $<\vec{x}|\vec{y}|VP|\phi>$ separately. Thus $tP\phi$ will be decomposed into $VP\phi + rP\phi$. One obtains

$$<\vec{x}|\vec{y}|VP|\phi> = \sum_{\lambda} \sum_{LM} Y_{L,M}^{L,M}(\vec{x}, \vec{y}) \sqrt{2}\delta_{M,m_0}(-)^{l_o}V(x)$$

$$\sum_{\lambda_0} i^{\lambda_0}\sqrt{2\lambda_0 + 1}C(l_0\lambda_0 L; m_0, 0)$$

$$\sum_{k} \sqrt{2k + 1}(-)^{k} A_{kL}^{L,M}(x, y) \left[1 + (-)^{\lambda_0+\lambda+k}\right]$$

$$\int_{-1}^{+1} dt P_k(t) u_{n_0}(\frac{1}{2}x + \vec{y}) j_{\lambda_0}(q_0)(\frac{3}{4}x - \frac{1}{2}\vec{y}),$$

(107)

where $A$ is given by (see Appendix B)

$$\int d\vec{x} d\vec{y} Y_{L,M}^{L,M}(\vec{x}, \vec{y}) Y_{k,k}^{0,0}(\vec{x}, \vec{y}) Y_{0,0}^{L,M}(\frac{1}{2}x + \vec{y}, \frac{3}{4}x - \frac{1}{2}\vec{y})$$

$$= \delta_{L,L,L} \delta_{M,m_0} A_{k,L}^{L,M}(x, y).$$

(108)

Now the projection onto the orthogonal states $Y_{L,M}^{L,M}(\vec{x}, \vec{y})$ defines $T_{L,M}^{0,1}(x, y)$

$$T_{L,M}^{0,1}(x, y) \equiv \int d\vec{x} d\vec{y} Y_{L,M}^{L,M}(\vec{x}, \vec{y}) T_{L,M}^{0,1}(\vec{x}, \vec{y})$$

(109)

in terms of which we obtain the two pieces of the driving term $T_{L,M}^{0,1}$

$$T_{L,M}^{0,1}(xy) = \frac{2\sqrt{2}}{\pi} \left(\frac{4}{3}\right)^{\lambda} ((-)^{l_o} + (-)^{l}) \delta_{M,m_0}$$

$$\int_{0}^{\infty} dq q^2 j_{\lambda}(qy) \int_{0}^{\infty} dy' y'^2 \int_{0}^{\infty} dy'' y'^2 j_{\lambda}(qy')$$

$$\sum_{k} \sqrt{k}(-)^{k} \sum_{\lambda_0} i^{\lambda_0+\lambda_0} j_{\lambda_0}(q_0 y''') \sqrt{\lambda_0}$$

$$h_{kL}^{L,L}(y', y'') C(l_0\lambda L, m_0, 0)$$

$$\int_{-1}^{1} dt P_k(t) r_{l}(x, |\frac{1}{3} y'''| + \frac{2}{3} |y'|; \epsilon_q) u_{n_0}(\frac{2}{3} y''' + |\frac{4}{3} y'|)$$

$$+ \sqrt{2}\delta_{M,m_0}(-)^{l_o}V(x) \sum_{\lambda_0} \sqrt{\lambda_0}$$

$$C(l_0\lambda L, m_0, 0) \sum_{k} \sqrt{k}(-)^{k} A_{kL}^{L,M}(x, y)$$

$$\int_{-1}^{1} dt P_k(t) u_{n_0}(\frac{1}{2}x + \vec{y}) j_{\lambda_0}(q_0)(\frac{3}{4}x - \frac{1}{2}\vec{y})(1 + (-)^{\lambda_0+\lambda+k})$$

Here and in the following we use the notation $\hat{s} \equiv 2s + 1$. This symbol $\hat{s}$ should of course not be confused with the unit vector.

Before addressing the second part of the driving term in Eq. (11) or (76) connected to the 3-atom force we regard the part of the kernel without 3-atom force, $<\vec{x}|\vec{y}|tG_0 PT>$ . Using similar steps and projecting onto states of total angular momentum $L$ leads to

$$K_{L}^{(1)}(xy) \equiv \int d\vec{x} d\vec{y} Y_{L,M}^{L,M}(\vec{x}, \vec{y}) <\vec{x}|\vec{y}|tG_0 PT>$$

$$= 4 \int_{0}^{\infty} dq q^2 j_{\lambda}(qy) \int_{0}^{\infty} dx' x'^2 \int_{0}^{\infty} dx'' x''^2 n(x, x'; \epsilon_q) g_l(x', x''; \epsilon_q)$$

$$\int_{0}^{\infty} dy'' y'^2 j_{\lambda}(qy'') \sum_{\lambda'\lambda} \sum_{k} \sqrt{k}(-)^{k} A_{kL}^{L,M}(x', y'')$$

$$\int_{-1}^{1} dt P_k(t) T_{L,L}(\frac{1}{2}x'' + \vec{y}', |\frac{3}{4} x'' - \frac{1}{2} y''|)(1 + (-)^{X+\lambda})$$

(111)
where we have defined the quantities \( T_{l\alpha l} \) in terms of the expansion

\[
T(\bar{x}, \bar{y}) \equiv \sum_{l\lambda l M} Y_{l\alpha l}^{M}(\bar{x}, \bar{y}) T_{l\alpha l}(xy)
\]

(112)
of \( T(\bar{x}, \bar{y}) \) given in Eqs. (11) and \( (177) \). We see that the unknown amplitudes \( T_{l\alpha l}(xy) \) occur under the integral with shifted arguments.

Next we expand the 3-body force of

\[
\frac{4\pi}{(2\pi)^{3/2}} \sum_{\lambda_0} i^{\lambda_0} \left( \frac{\lambda_0}{4\pi} j_{\lambda_0}(q_0 y) u_n(x) V^{(1)}(xy \cdot \bar{y}) \right)
\]

(113)
and project \((115)\) onto \( Y_{l\alpha l}^{M}(\bar{x}, \bar{y}) \) explicitly. We expand the plane wave and introduce states of total angular momentum, with the result

\[
< \bar{x}, \bar{y} | V^{(1)} | \phi_1 > = \frac{4\pi}{(2\pi)^{3/2}} \sum_{\lambda_0} i^{\lambda_0} \left( \frac{\lambda_0}{4\pi} j_{\lambda_0}(q_0 y) u_n(x) V^{(1)}(xy \cdot \bar{y}) \right)
\]

Next we expand the 3-body force \( V^{(1)} \) into Legendre polynomials

\[
V^{(1)}(x, y, \bar{x} \cdot \bar{y}) = \sum_{k} 2\pi \sqrt{k} (-)^k Y_{kk}^{L M_0}(\bar{x}, \bar{y}) v_k
\]

(114)
with

\[
v_k(x, y) = \int_{-1}^{1} dt P_k(t) V^{(1)}(x, y, \bar{x} \cdot \bar{y})
\]

(115)
and combine the angular dependent terms as

\[
Y_{kk}^{L M_0}(\bar{x}, \bar{y}) Y_{l\alpha l}^{M}(\bar{x}, \bar{y}) = \frac{1}{4\pi} \sqrt{k_0 l_0 \lambda_0 (-)^{\lambda_0 + L + k}} \sum_{\mu_1 \mu_2} \left( (-)^{\mu_1} \left\{ \begin{array}{c} \mu_1 \\ \lambda_0 \\ l_0 \end{array} \right\} \right) C(k l_0 \mu_1, 00) C(k \lambda_0 \mu_2, 00) Y_{l\alpha l}^{M}(\bar{x}, \bar{y})
\]

(116)
where the terms in curly bracket are 6-j symbols. Finally projecting Eq. (113) onto \( Y_{l\alpha l}^{M}(\bar{x}, \bar{y}) \) one obtains

\[
\int d\bar{x} \int d\bar{y} Y_{l\alpha l}^{M*}(\bar{x}, \bar{y}) < \bar{x}, \bar{y} | V^{(1)} | \phi > = \frac{1}{2\sqrt{2\pi}} \sum_{\lambda_0} i^{\lambda_0} \lambda_0 j_{\lambda_0}(q_{0y}) u_{n0}(x) \sum_{\kappa} k \sqrt{i_{0}(-)^{\lambda_0 + L + l}} \left\{ \begin{array}{c} l \\ \lambda_0 \\ l_0 \end{array} \right\} C(k l_{0} l_{1}, 00) C(k \lambda_{0} \mu_{2}, 00) C(l_{0} \lambda_{0} L, m_{0}, 0)
\]

(117)
\[
\delta_{M, M_0} \int_{-1}^{1} dt P_k(t) V^{(1)}(x, y, t)
\]
The other pieces of that second part of the driving term can be worked out similarly and we obtain altogether

\[
T_{l\alpha l}^{02}(xy) = \int_{0}^{\infty} dx' x'^{2} \int_{0}^{\infty} dy' y'^{2} \left[ \frac{\delta(x - x')}{xx'} \right] \left[ \frac{\delta(y - y')}{yy'} \right] \int_{0}^{\infty} dq dq' j_{l}(q y) j_{l}(q y') \int_{0}^{\infty} dx'' x''^{2} \tau_{l}(x''; \epsilon_{q}) g_{l}(x''; \epsilon_{q'})
\]

(118)
\[
+ \left( \frac{1}{2\sqrt{2\pi}} \sum_{\lambda_0} i^{\lambda_0} \lambda_0 j_{\lambda_0}(q_{0y}) u_{n0}(x') \sqrt{i_{0}(-)^{\lambda_0 + L + l}} \left\{ \begin{array}{c} l \\ \lambda_0 \\ l_0 \end{array} \right\} C(k l_{0} l_{1}, 00) C(k \lambda_{0} \mu_{2}, 00)
\]

\[
+ (-)^{l_0} \sum_{k} \int_{-1}^{1} dt P_{k}(t) u_{n0}(x') \left( \frac{1}{2} x'' + \frac{1}{2} y'' \right) j_{l}(q_{0y}) \frac{3}{4} x'' - \frac{1}{2} y''
\]

\[
+ \sum_{\mu} \left( \frac{(-)^{\mu}}{\sqrt{\mu}} C(k k' \mu, 00)^{2} \Lambda_{l', l_{1}, 0}^{\mu l} (x' y')(1 + (-)^{\lambda_0 + l_{1} + \mu + k'})
\]
The remaining parts of the kernel in Eq(11) or (77) can be worked out similarly and we split it into two pieces:

\[
K^{(2,1)}_{\lambda L}(xy) = \int \frac{d\hat{x}}{2\pi} \int \frac{d\hat{y}}{2\pi} Y_{\lambda}^{L\ast M}(\hat{x}\hat{y}) < \hat{x}\hat{y}|V^{(1)}G_0(1 + P)T > \\
= \frac{1}{\pi} \sum_{k} k(-k) \int_{-1}^{1} dtV^{(1)}(x,y,t) \sum_{\nu_2} \int_{0}^{\infty} dq q^2 j_{\nu_2}(qy) \\
\sum_{\mu_1} \sqrt{\mu_1\mu_2} (-l)^{\mu_2+k+l} \left\{ \begin{array}{ccc} l & \lambda & L \\ \mu_2 & \mu & k \end{array} \right\} C(k\mu_1l,00)C(k\mu_2\lambda,00) \\
\int_{0}^{\infty} dx x^2 \int_{0}^{\infty} dy y^2 j_{\mu_2}(qy)g_{\mu_2}(xx',\epsilon_q)|T_{\mu_1\mu_2L}(x'y') > \\
+ \sum_{k'} (2\pi) \sqrt{k'} (-k') \sum_{l'\lambda'} \int_{-1}^{1} dtP_{k'}(t)|T_{l'\lambda'}L|(1 \frac{1}{2} x'' + \hat{y}'|,| \frac{3}{4} x'' - \frac{1}{2} \hat{y}>) \\
\quad (-l')^2 + (-l')^2 + \lambda' \mu_2)A_{k'\mu_1L,l'\lambda'}(x'y')
\]

and

\[
K^{(2,2)}_{\lambda L}(xy) = \int \frac{d\hat{x}}{2\pi} \int \frac{d\hat{y}}{2\pi} Y_{\lambda}^{L\ast M}(\hat{x}\hat{y}) < \hat{x}\hat{y}|t_1G_0V^{(1)}G_0(1 + P)T > \\
= \frac{2}{\pi} \int_{0}^{\infty} dq q^2 j_{\lambda}(qy) \int_{0}^{\infty} dy y^2 j_{\lambda}(qy') \int_{0}^{\infty} dx x^2 dx' dx'' \\
\tau_l(x''x';\epsilon_q)g_l(x''x';\epsilon_q)K^{(2,1)}_{\lambda L}(x'y')
\]

Then we end up with the one integral equation for \(T_{\lambda L}(xy)\) in the form

\[
T_{\lambda L}(xy) = T^{0,1}_{\lambda L}(xy) + T^{0,2}_{\lambda L}(xy) + K^{(1)}_{\lambda L}(xy) + K^{(2,1)}_{\lambda L}(xy) + K^{(2,2)}_{\lambda L}(xy)
\]

where the \(T^{0,i}\) are the driving terms and the \(K\)’s incorporate the \(T\)-amplitudes.

These are coupled equations among the \(T\)’s, since Eqs (11), (19) and (20) contain sums over several \(T\)’s. Once the \(T\)-amplitudes in case of distinguishable particles are obtained we can use the Eqs. (26), (27), (28) to determine the elastic and arrangement amplitudes as well as the complete break-up amplitude (20). In the case of identical atoms one can not distinguish, of course, between elastic and arrangement amplitudes. Let us first regard the elastic amplitude given in Eq(13).

For \(< \phi'|PT|\phi >\) one expands the plane wave, introduces the expression (112) for \(T\), total angular momentum states and finally expands \(u_{m'}((\frac{1}{3} \hat{y}' + \frac{2}{3} \hat{y})T_{\lambda L}(\frac{1}{3} \hat{y}' + \frac{2}{3} \hat{y},y'))\) into Legendre polynomials. Then the same expression (105) for the remaining angular integrations appears and we obtain

\[
< \phi'|PT|\phi > = 2\sqrt{2\pi}(\frac{4}{3})^3 \sum_{\lambda'} \lambda! Y_{-m_0-m'}(\hat{q}') \\
\int_{0}^{\infty} dy y^2 \int_{0}^{\infty} dy y'^2 \sum_{l'\lambda'} C(l'\lambda' L, m' m_0 - m') \sum_{k} \sqrt{k} (-k)^k \\
\sum_{l\lambda} h_{l\lambda}^{(k)}(y,y')((-)^l + (-)^{l'}) \\
\int_{-1}^{1} dtP_k(t)u_{m'}((\frac{4}{3} \hat{y}' + \frac{2}{3} \hat{y})T_{l\lambda L}(\frac{2}{3} \hat{y}' + \frac{4}{3} \hat{y},y'))
\]

Here \(m'\) is the magnetic quantum number of the final 2-atom bound state with orbital angular momentum \(l'\) and \(h_{l\lambda}^{(k)}\) has been defined previously in (105).
Very similar steps applied to $<\phi'|PG_0^{-1}\phi>$ lead to

$$<\phi'|PG_0^{-1}\phi> = \frac{2}{\sqrt{\pi}} \left(\frac{4}{3}\right)^3 \sum_{\lambda'} (-i)^{\lambda'} Y_{\lambda' m_0 - m'}(\hat{q}') \int dyy^2 \int dy'y'^2 \sum_{\lambda_0} \phi_0^{(j_{\lambda'}(q'y))} j_{\lambda_0}(g_0 g') \sqrt{\lambda_0}(-)^{l_0} + (-)^{l'}$$

$$\sum_{L} C(l'\lambda' L, m'm_0 - m') C(l_0\lambda_0 L, m_0, 0) \sum_{k} \sqrt{k} (-)^k h_{k_{\lambda', \lambda}}^{(L)}(y, y') \int dt P_k(t) u_{m'}(\frac{1}{3} y' + \frac{2}{3} g) V(\frac{1}{3} y' + 4\frac{2}{3} g) u_{m}(\frac{1}{3} y' + 4\frac{2}{3} g)$$

There are two more terms in Eq. (13) which are worked out by similar steps as for the kernel parts. The resulting expressions are

$$<\phi'|V^{(1)}(1 + \mathcal{P})\phi> = \frac{(-)^{l_0}}{\sqrt{2}} \sum_{\lambda'} \sum_{\lambda_0} \phi_0^{l_0} j_{\lambda'}(q'y) j_{\lambda}(q'y) \int dyy^2 \int dx x^2 \int dy y^2 \sum_{\lambda} C(l_0 \lambda_0 L, m_0, 0) C(l'\lambda' L, m'm_0 - m')$$

$$\sum_{k} \sqrt{k} (-)^k \int dt P_k(t) V^{(1)}(xyt)$$

$$\left[ \frac{1}{2\pi} \int_{l_0}(\hat{q}) \sqrt{\lambda_0} j_{\lambda_0}(g_0 g) u_{m_0}(x)(-)^{l'} \{ \begin{array}{c} \lambda' \lambda_0 \lambda_0 \lambda'_0 \lambda_0 \end{array} \} C(k \lambda_0 L, 0) C(k \lambda_0 L', 0)$$

$$+ \sum_{k'} \sqrt{k'} (-)^{k'} \int dt P_{k'}(t) u_{m_0}(\frac{1}{2} x + \frac{1}{2} y) j_{\lambda_0}(g_0(\frac{3}{4} x - \frac{1}{2} y))$$

$$\sum_{\lambda} \int dyy^2 j_{\lambda}(q'y)$$

$$\sum_{l_0} \sqrt{\mu_{l_0}} (-)^{l_0 + \lambda + \lambda'} C(k \mu_{l_0} L, 0) C(k \mu_{l_0} L', 0)$$

$$\int_{0}^{\infty} dx x^2 \int_{0}^{\infty} dy y^2 j_{\mu_2}(q'y) g_{1}(xx', \epsilon_q) [T_{l_0 l_2 L}(x'y')]$$

$$+ \sum_{l'} \sum_{l''} (2\pi) \sqrt{k''} (-)^{l''} \sum_{l', L} \int dt P_{k''}(t) T_{l'\lambda' L}(\frac{1}{2} x' + \frac{1}{2} y', \frac{3}{4} x' - \frac{1}{2} y')$$

Finally the complete break-up amplitude $<\phi_0|(1 + \mathcal{P})T>$ according to Eq. (12) can be based on its first term

$$T(p q) \equiv <\phi_0|T> \equiv <\hat{p} q|T>$$

$$= \frac{1}{(2\pi)^{3/2}} \int dx dy e^{-i p \cdot x} e^{-i q \cdot y} \sum_{l' \lambda' L'} \mathcal{J}_{l' \lambda' L'}^{(m_0)}(\hat{x} \hat{y}) T_{l' \lambda' L'}(xy)$$
Expanding the plane waves one readily obtains

$$T(\vec{p}\vec{q}) = \frac{2}{\pi} \sum_{\alpha, \lambda} Y^{\alpha \lambda \mu}_L(\vec{p}\vec{q})(-i)^{\lambda+\mu} \int_0^\infty dx x^2 \int_0^\infty dy y^2 j_0(px)j_\lambda(qy)T_{\alpha\lambda}(xy)$$

(127)

The remaining two terms in integral equation (121) composed of the parts (110), (118), (111), (119) and (120) now reads

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

$$\frac{1}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

This concludes the display of the formalism. The cases for two identical atoms out of the three or three distinguishable atoms are somewhat more tedious to be worked out, but straightforward and are left to the interested practitioner.

V. THE S-WAVE EXPRESSIONS

For very low energy of the incoming atom and the molecule in its ground state one can restrict the treatment to setting all orbital angular momenta to zero. Then the final expressions simplify and allow an overview of the structure of the integral equation to be solved and the quadrature expression for elastic scattering. Again we display only the case of identical atoms. In this case the quantities \( \Lambda \) and \( h \) given in the Appendices both simplify to \( \frac{1}{\pi} \) and the integral equation (121) composed of the parts (110), (118), (111), (119) and (120) now reads

$$T_{000}(x, y) = \frac{\sqrt{2}}{\pi^2} \frac{1}{3} \int_0^\infty dq dq' j_0(qy) \int_0^\infty dy' y' j_0(qy') \int_0^\infty dy'' y'' j_0(qy'') \int_0^\infty \frac{dx x^2}{\sqrt{2\pi}} \left[ \int_0^1 dt \left[ \frac{1}{2} x \left( \frac{1}{2} x + y \right) \right] u_{\alpha\lambda}(x) \right] + \frac{1}{2} \int_0^\infty dq dq' j_0(qy) j_0(qy') \int_0^\infty dx' x'^2 \int_0^\infty dy' y'^2 \frac{\delta(x-x')}{xy} \frac{\delta(y-y')}{yx'}$$

(128)
The elastic amplitude given by the expressions (119), (121), (122), (123) also simplifies and one obtains

\[
< \phi'|U|\phi > = \frac{1}{2\pi^2} \int_0^\infty dyy^2 \int_0^\infty dy'|y'^2 j_{\lambda'}(q'y')j_0(q_0y')
\]

\[
\int_{-1}^1 dtu_{n_0}(\frac{4}{3}y' + \frac{2}{3}y)V(\frac{2}{3}y' + \frac{4}{3}y)u_{n_0}(\frac{2}{3}y' + \frac{4}{3}y)
\]

\[
+ \frac{\sqrt{2}}{2\pi} (\frac{3}{4}) \int_0^\infty dyy^2 \int_0^\infty dy'|y'^2 \int_{-1}^1 dtu_{n_0}(\frac{4}{3}y' + \frac{2}{3}y)T_{000}(\frac{2}{3}y' + \frac{4}{3}y), y')
\]

\[
+ \frac{1}{2} (2\pi)^{3/2} \int_0^\infty dxx^2 \int_0^\infty dyy^2 u_{n_0}(x)j_0(q'y') \int_{-1}^1 dtV^{(1)}(xy,t) [j_0(q_0y)u_{n_0}(x)j_0(q_0y)j_0(3x^2 - 1)\frac{1}{2}y]
\]

\[
+ \frac{1}{2\sqrt{2} \pi^2} \int_0^\infty dxx^2 \int_0^\infty dyy^2 u_{n_0}(x)j_0(q'y') \frac{1}{\sqrt{4\pi}} \int_{-1}^1 dtV^{(1)}(xy,t) \int_0^\infty dqq^2 j_0(qy)
\]

\[
\int_0^\infty dxx'x'^2 \int_0^\infty dyy'^2 j_0(q'y')g_0(xx';\epsilon_q)
\]

\[
[T_{000}(x'y') + \int_{-1}^1 dtT_{000}(\frac{1}{2}x^2 + \frac{3}{4}\frac{1}{2}y', |\frac{3}{4}\frac{1}{2}y' - \frac{1}{2}|)]
\]

At this low energy complete break up will not be possible.

VI. COMPUTATIONAL CONSIDERATIONS

The numerical solution of the integral equations for the T-amplitudes requires a large amount of computer time, depending on the number of angular momenta that enter in the partial wave expansion, and also on the number of mesh points that are needed for the discretization of the integration kernels, or equivalently, on the number of mesh points needed for the discretization of the coordinates x and y. We expect to minimize the number of required mesh points by using a recently developed spectral integral equation method (S-IEM) for solving the two-body Lippmann-Schwinger integral equation in configuration space that is very economical in the number of mesh points required for a given accuracy. This feature has now been demonstrated in several applications that are summarized in [4]. For example [7], for the case of the binding energy of the He-He dimer which is very small, the calculation of the bound state wave function has to be carried out to large distances. For a distance of 3000 a.u. the S-IEM required only 200 mesh points to obtain an accuracy of three significant figures for the binding energy, and with 320 mesh points the accuracy increased to six significant figures [6]. The method consists in dividing the radial interval into partitions, each partition receiving a fixed number of mesh points, expanding the unknown wave function into a series of Chebyshev polynomials in each partition, and then solving for the coefficients of the expansion. Such expansions are by themselves very efficient, and their accuracy properties are known. In addition, the size of the partitions is made automatically small in the region where the wave function changes rapidly, and large where it changes slowly, a feature that further contributes to the economy. An additional advantage of the spectral method is that conventional interpolation methods can be avoided. In the Faddeev scheme the Jacobi coordinates in one arrangement have to be translated into the corresponding coordinates in another arrangement. These translated points do not fall onto the predetermined mesh of points in another arrangement, hence interpolations are usually required with methods using fixed mesh points. The spectral method avoids this problem, since the Chebyshev polynomials, being analytic functions, can be evaluated at any prescribed positions, and hence provide the necessary translations.

The two-body \( \tau \) - matrices play a large role in the calculation of the driving terms (116), (117) and the integration kernels (118), (119), (120). Investigations in progress are showing that the S-IEM can also be applied to the evaluation of the two-variable \( \tau \) - matrices, and the partition structure of the radial intervals of the latter will then subsequently determine the partition structure of the integration kernels. The number of mesh points for each of the two variables in the \( \tau \)-matrix is expected to be of the order of 50. The size of the matrices that represent the integration kernels will have to be estimated, and depending on the outcome, iterative procedures may be required.
VII. SUMMARY AND CONCLUSIONS

The purpose of this paper is to lay out the theoretical formulation of the solution of the three-body Faddeev integral equations in configuration space, for the purpose of applying them to atomic physics situations. It is assumed that the Born-Oppenheimer approximation is valid and the three atoms are moving on one potential surface. The case of a conical intersection is not treated but it appears conceivable that also such a case could be handled by using coupled Faddeev equations, similar to the treatment of $\Delta$-excitations in a three-nucleon problem. We have chosen a formulation of the Faddeev equations which turned out to be extremely useful in nuclear physics [1]. Instead of working with wave function components we introduce break-up amplitudes $T_i$, which vanish at large distances and fulfill a set of three coupled equations. In case of identical atoms only one equation is needed. That set of equations is then displayed in a configuration space vector representation and further decomposed into partial waves. For the sake of clarity this set of coupled equations is also presented assuming s-waves only. Once the T-amplitudes are determined all physical matrix elements for elastic and inelastic atom-diatom scattering, for the arrangement processes and the complete 3-atom break-up process are obtained by simple quadrature. The relevant expressions are given in detailed form.

One reason for working in configuration space is that the atom-atom two- and three-body potential surfaces are given in that space. One objection commonly raised against performing three-body calculations in configuration space is that one needs many mesh points for the numerical implementation, because the wave functions have to be calculated out to large distances in order to impose the asymptotic boundary conditions. We overcome this objection for several reasons. One is, as already said, that we do not calculate wave functions, but rather T-amplitudes. These functions are essentially the product of wave functions times potentials, and hence decay fast with distance in contrast to wave functions, which oscillate at infinity. Also, the asymptotic boundary conditions of the underlying wave functions are automatically included, because the Faddeev integral equations contain the Greens functions which lead to the appropriate asymptotic behavior. Another objection against working in configuration space is that wave functions, and so also T-amplitudes, can have a strongly oscillatory behavior, and hence many mesh points may be required. We expect to overcome this objection by using a recently developed spectral method (S-IEM) for solving the two-body Lippmann-Schwinger integral equation that is very economical in the number of mesh points required for a given accuracy [4]. The economy in mesh points is crucial when solving the Faddeev integral or differential equations, because the numerical complexity increases like the cube of the dimension of the final matrix, and the size of the dimension is proportional to the number of mesh points.

In summary in this paper we lay out in detail the partial wave expanded Faddeev equations for the $T$-amplitudes in configuration space and in integral form. These equations, although complicated, are not much more complicated than the corresponding equations in momentum space, which have been successfully solved in the realm of nuclear physics. In a future study we intend to solve the equations for a simple test case in order to study the numerical feasibility of the method.

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APPENDIX A: THE EXPRESSION $h_{k,L}^{k,L}(y,y')$ FROM EQ(105)

The evaluation of $h$ can be done using standard angular momentum algebra [5] [6]. So we do not provide the detailed steps but mention only some useful formulas, which are needed and possibly not so commonly in use.

The dependence on the two vector directions in the shifted arguments for the spherical harmonics can be separated using

$$Y_{lm}(\vec{a} + \vec{b}) = \sum_{l_1+l_2=l} \frac{a^{l_1} b^{l_2}}{|\vec{a} + \vec{b}| l} \sqrt{\frac{4\pi (2l+1)!}{(2l_1+1)!(2l_2+1)!}} Y_{lm}^{l_1 l_2} (\vec{a}, \vec{b})$$

(A1)
Further in the course of recoupling the following formula is needed

$$\mathcal{Y}_{i_1 i_2}^{l m} (\hat{a}, \bar{\alpha}) = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} C(l_1 l_2 l, 00) Y_{l m}^{(\bar{a})}$$  \hspace{1cm} (A2)$$

The resulting expression for $h$ is

$$h_{i_1 i_2}^{k, L_{\lambda}}, (y, y') = \int d\hat{y} \int d\hat{y}' \mathcal{Y}_{i_1 i_2}^{L_{\lambda}, \lambda} (\hat{y}, \bar{\lambda}) \mathcal{Y}_{k, k}^{0, 0} (\hat{y}, y') \mathcal{Y}_{\alpha, \alpha}^{L_{\mu}, \mu} (\frac{2}{3} \hat{y} + \frac{4}{3} \bar{\lambda}, \bar{\lambda})$$  \hspace{1cm} (A3)$$

$$= \frac{1}{8\pi} \sum_{l_1 + l_2 = l} \sum_{l_1' + l_2' = l'} y^{l_1 + l_1' y^{l_2 + l_2'}} (\frac{2}{3})^{l_1 + l_1'} (\frac{4}{3})^{l_2 + l_2'}$$  \hspace{1cm} (A4)$$

APPENDIX B: THE EXPRESSION $A_{i_1 i_2}^{k, L_{\lambda}}, (xy)$ FROM EQ (108)

$$A_{i_1 i_2}^{k, L_{\lambda}}, (xy) = \int \mathcal{Y}_{i_1 i_2}^{L_{\lambda}, \lambda} (\hat{x}, \bar{\lambda}) \mathcal{Y}_{k, k}^{0, 0} (\hat{x}, y) \mathcal{Y}_{\alpha, \alpha}^{L_{\mu}, \mu} (\frac{1}{2} \hat{x} + \hat{y}, \frac{3}{4} \bar{x} - \frac{1}{2} \bar{y})$$  \hspace{1cm} (B1)$$

$$= \frac{1}{8\pi} \sum_{l_1 + l_2 = l} \sum_{l_1' + l_2' = l'} \frac{1}{4} \lambda^{l_1 + l_1'} \left( \frac{3}{4} \right)^{l_1} \left( \frac{3}{4} \right)^{l_1} \left( - \right)^{l_1} \left( x_{l_1} x_{l_1'} y_{l_1} y_{l_1'} \right)$$  \hspace{1cm} (B2)$$

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