J Math Chem (2015) 53:1426–1444
DOI 10.1007/s10910-015-0497-3

ORIGINAL PAPER

Three-particle integrals with spherical Bessel and Neumann functions and photodetachment of the negatively charged hydrogen ions

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Received: 17 February 2015 / Accepted: 23 March 2015 / Published online: 31 March 2015

Abstract A few approaches are derived to calculate three-particle integrals which include spherical Bessel functions of the first and second kind, i.e., the $j_\ell(Vr)$ and $n_\ell(Vr)$ functions. Such integrals are important in applications to various problems known in atomic and nuclear physics. In particular, these integrals are needed in accurate computations of the photodetachment cross-section(s) of negatively charged hydrogen ions.

Keywords Three-particle · Integrals · Bessel functions · Photodetachment

1 Introduction

In different areas of physics there are real situations where one (or few) particles in a few-body system becomes free after some 'fast' process in the originally stable system. For instance, the non-relativistic photodetachment of the negatively charged hydrogen ion H^-, leads to the formation of the neutral hydrogen atom H and one 'free' electron (emitted photo-electron). Such an electron can be considered as a free electron, if we can neglect its interaction with the final (neutral) atom. Numerical calculations of the final state probabilities are reduced to computations of some three-particle integrals which include spherical Bessel functions of the first and second kind.

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Another example is the formation of the protium and tritium atoms during the (^{3}He, n; p, t)-nuclear reaction. This reaction is highly exothermic ($\Delta E \approx 0.764$ MeV). The energy released during this reaction accelerates two final nuclei (protium and tritium) to relatively high velocities, which are larger than regular atomic velocities v_a [1]. The formation of final atoms/ions also leads to computations of integrals which include Bessel functions. The same integrals arise during calculations of the final state probabilities in atoms/molecules undergoing the nuclear $\beta^{\pm}$-decay.

To define three-particle integrals which include spherical Bessel functions let us discuss the problem of atomic photodetachment. In the middle of 1940's Chandrasekhar tried to develop an effective procedure to calculate the photodetachment cross-section of the negatively charged hydrogen H^- ion [2–4], i.e. the cross-section of the process $H^- + \hbar\omega = H + e^-$. In his calculations he applied accurate variational wave functions of the H^- ion which had become avaliable at that time which reduced the original problem to calculations of the following integral

$$\int_0^{+\infty}\int_0^{+\infty}\int_{|r_2-r_1|}^{r_2+r_1} \exp(-\alpha r_2 - \beta r_1) j_1(K r_2) r_2^{n_1} r_1^{n_2} r_{21}^{n_3} dr_2 dr_1 dr_{21} \tag{1}$$

where $j_1(x) = \frac{sinx}{x^2} - \frac{cosx}{x}$ is the Bessel function of the first kind. Also, in Eq. (1) and below α, β are the positive real numbers, while n_1, n_2, n_3 are the non-negative integer numbers. To determine the integral, Eq. (1), Chandrasekhar used an approximate numerical method, since closed analytical formulas for integrals similar to the integral defined in Eq. (1) were not known.

Later similar integrals we found in various few-body problems. Finally, we need to consider the problem of analytical and numerical calculations of three-particle integrals which include spherical Bessel functions of the first and second kind, i.e., the $j_\ell(Vr)$ and $n_\ell(Vr)$ functions. The general three-particle integral with the spherical Bessel function $j_L(kr_{32})$ is defined in the following form

$$\mathcal{J}_L(\alpha, \beta, \gamma; n_1, n_2, n_3) = \int_0^{+\infty}\int_0^{+\infty}\int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) j_L(K r_{31}) \times r_{32}^{n_1} r_{31}^{n_2} r_{21}^{n_3} dr_{32} dr_{31} dr_{21} \tag{2}$$

where n_i ($i = 1, 2, 3$) are integer non-negative numbers. This form of the three-particle integral is more general than defined by Eq. (1). Formally, Eq. (2) can be considered as the 'three-dimensional' Laplace transform of the Bessel function $j_L(K r_{31})$. However, such a definition of Laplace transform leads to a number of problems, since three relative coordinates r_{32}, r_{31} and r_{21} are not truly independent (see discussion below).

General three-body integrals with the spherical Neumann function $n_L(kr_{31})$ are defined analogously [5], i.e.

$$\mathcal{N}_L(\alpha, \beta, \gamma; n_1, n_2, n_3) = \int_0^{+\infty}\int_0^{+\infty}\int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) n_L(K r_{31}) \times r_{32}^{n_1} r_{31}^{n_2} r_{21}^{n_3} dr_{32} dr_{31} dr_{21} \tag{3}$$

where α, β, γ are the varied, non-linear parameters (real numbers). In Eqs. (2)–(3) the three variables r_{32}, r_{31} and r_{21} are scalar interparticle distances $r_{ij} =\mid \mathbf{r}_i - \mathbf{r}_j \mid = r_{ji}$, which correspond to the sides (or ribs) of the triangle formed by the three particles 1, 2 and 3. Note that the three relative coordinates are not completely independent of each other, since, e.g., $r_{21} \le r_{32} + r_{31}$ and $r_{21} \ge \mid r_{32} - r_{31} \mid$ and this complicates analytical and numerical computations of the three-body integrals in the relative coordinates. To avoid numerous problems which follow from partial dependence of the relative coordinates, in our earlier works we have used three perimetric coordinates u_1, u_2, u_3 which can be expressed as linear combinations of the three relative coordinates r_{32}, r_{31} and r_{21} (see, e.g., [6]). The three perimetric coordinates u_1, u_2, u_3 are independent of each other and each of them changes between 0 and $+\infty$. This approach is very general and quickly leads to closed analytical expressions for the integrals Eqs. (2)–(3) with different powers of three variables r_{32}, r_{31} and r_{21}. However, for certain types of three-particle integrals, e.g., for integrals in which the function $F(r_{32}, r_{31}, r_{21})$ depends upon one relative coordinate only, the methods based on the perimetric coordinates are too complex and not very effective in applications. It is clear that in such cases we need to develop more effective and direct methods for calculations of three-body integrals in which $F(r_{32}, r_{31}, r_{21}) = f(r_{32})$, where $f(r_{32})$ can also be equal to the $j_L(r_{32})$ and/or $n_L(r_{32})$ functions. With such methods in hand one can say that the original problem is solved completely and accurately.

Let us discuss another approach which is based on the direct integration of Eqs. (2)–(3) in the relative coordinates. This approach is not universal and it can be applied only in those cases when the function $F(r_{32}, r_{31}, r_{21})$ depends upon one relative coordinate only. Below, without loss of generality, we shall assume that $F(r_{32}, r_{31}, r_{21}) = f(r_{32})$. In this case the three-particle integral is written in the form

$$I(\alpha, \beta, \gamma; f) = \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} f(r_{32}) \times \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) r_{32} r_{31} r_{21} dr_{32} dr_{31} dr_{21} \quad (4)$$

or, we can write:

$$I(\alpha, \beta, \gamma; f) = -\frac{\partial^3}{\partial\alpha\partial\beta\partial\gamma} J(\alpha, \beta, \gamma; f) \quad (5)$$

where

$$J(\alpha, \beta, \gamma; f) = \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} f(r_{32}) \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) dr_{32} dr_{31} dr_{21} \quad (6)$$

Three-particle integrals, Eq. (4), arise in various three- and few-body problems, e.g., when the exponential variational expansion in the relative (or perimetric) coordinates is used to approximate wave functions of the incident (bound) state and the second particle becomes unbound during such a process. In general, such an expansion is very effective in actual bound state calculations, since it is compact and accurate at the same time (for more detail, see, [7,8] and references therein).

The first approach developed in this study for calculations of the three-particles integrals, Eq. (4), is based on the following analytical formula for the integral $J(\alpha, \beta, \gamma; f)$, Eq. (6):

$$
\begin{aligned}
J(\alpha, \beta, \gamma; f) &= \frac{2}{\beta^2 - \gamma^2} \Big\{ \int_0^{+\infty} f(r_{32}) \exp[-(\alpha + \beta) r_{32}] dr_{32} \\
&\qquad - \int_0^{+\infty} f(r_{32}) \exp[-(\alpha + \gamma) r_{32}] dr_{32} \Big\} \\
&= \frac{2}{\beta + \gamma} \Big[\frac{L_p(f; \alpha + \beta) - L_p(f; \alpha + \gamma)}{\beta - \gamma} \Big]
\end{aligned} \tag{7}
$$

where it is assumed that $\beta \neq \gamma$. Formally, we can say that analytical computations of the $J(\alpha, \beta, \gamma; f)$ integrals, Eq. (6), are reduced to computations of the two Laplace transformations (L_p) of the function $f(x; s)$ with the two different exponents $s_1 = \alpha + \beta$ and $s_2 = \alpha + \gamma$. With the use of expression, Eq. (7), we can re-write the formula Eq. (5) in the form

$$
\begin{aligned}
I(\alpha, \beta, \gamma; f) &= -\frac{\partial^2}{\partial\beta\partial\gamma} \Big\{ \frac{2}{\beta^2 - \gamma^2} \Big[\frac{\partial L_p(f; \alpha + \beta)}{\partial\alpha} - \frac{\partial L_p(f; \alpha + \gamma)}{\partial\alpha} \Big] \Big\} \\
&= -\frac{\partial^2}{\partial\beta\partial\gamma} \Big\{ \frac{2}{\beta^2 - \gamma^2} \Big[L_p^{(\alpha)}(f; \alpha + \beta) - L_p^{(\alpha)}(f; \alpha + \gamma) \Big] \Big\}
\end{aligned} \tag{8}
$$

where $L_p^{(\alpha)}(f; \alpha + \beta) = \frac{\partial L_p(f; \alpha+\beta)}{\partial\alpha}$. Note that the term $L_p^{(\alpha)}(f; \alpha + \beta)$ does not depend upon the non-linear parameter γ, while the analogous term $L_p^{(\alpha)}(f; \alpha + \gamma)$ does not depend upon the non-linear parameter β. These two facts drastically simplify analytical computation of all derivatives with respect to the non-linear parameters β and γ in Eq. (8).

For the first time, one of us (AMF) derived the formulas, Eqs. (7)–(8) in the mid-1980's. Since then these formulas have been used in a number of applications, e.g., to derive analytical expressions for the matrix elements of some short-range potentials. It should be mentioned that applications of the formula, Eq. (7), are quite restricted, since the backward transition from Eq. (6) to Eq. (4) leads to numerical instabilities in the formulas arising in this approach. The source of such instabilities is clear, since the integral $J(\alpha, \beta, \gamma; f)$, Eq. (7), takes the form $\frac{0}{0}$, when $\beta \to \gamma$. A meaningful formula for the $\frac{0}{0}$ fraction can be obtained with the use of $L'H\hat{o}pital's$ rule, but then we need to calculate the partial derivatives of the third order from the arising expression. A general approach for calculations of such integrals is discussed in Sect. 2 below. In Sect. 3 we derive the explicit formulas for the integrals $J(\alpha, \beta, \gamma; f)$ which include the spherical Bessel and Neumann functions. Analytical computations of the derivatives of these formulas are considered in Sect. 4. Concluding remarks can be found in the last Section.

2 General approach

In those cases when $\beta = \gamma + \Delta$, where the value of Δ is relatively large, one can apply the formula, Eq. (8), directly. The arising formulas, however, cannot be used when $\beta \to \gamma$, or $\Delta \to 0$. Formally, even in such cases we can use Eq. (8), but its denominator contains the common factor Δ^3. Therefore, to produce some useful expression in the cases when $\beta \to \gamma$ and $\beta = \gamma$ we need to show that all terms in the numerator, which contains the factors Δ and Δ^2, are cancel each other. Moreover, to evaluate such expressions in those cases when $\Delta \approx 0$ we need to produce explicit formulas for the 'higher' terms with the factors Δ^4, Δ^5, etc. Practical experience indicates that the approach based on Eq. (8) is not an optimal way to derive the explicit formulas for the three-particle integrals. Instead, we can use a different approach.

Let us replace the two variables β, γ by the two new variables γ, Δ, where $\beta = \gamma + \Delta$. The variable Δ is assumed to be small in comparison with each of the β and γ variables. In these variables Eq. (8) takes the form

$$I(\alpha, \gamma+\Delta, \gamma; f) = -\frac{\partial^2}{\partial\gamma\partial\Delta}\left\{\frac{2}{2\gamma+\Delta} \cdot \frac{L_p^{(\alpha)}(f; \alpha+\gamma+\Delta) - L_p^{(\alpha)}(f; \alpha+\gamma)}{\Delta}\right\} \tag{9}$$

As one can see from this formula, in order to determine the integral $I(\alpha, \gamma+\Delta, \gamma; f)$ we need to derive the explicit formulas for the first four terms in the Taylor series of the $L_p^{(\alpha)}(f; \alpha+\gamma+\Delta)$ function (in terms of Δ):

$$L_p^{(\alpha)}(f; \alpha+\gamma+\Delta) = T_0 + T_1\Delta + T_2\Delta^2 + T_3\Delta^3 + \cdots \tag{10}$$

This allows one to write the following expression for the $I(\alpha, \gamma+\Delta, \gamma; f)$ integral

$$I(\alpha, \gamma+\Delta, \gamma; f) = -\frac{\partial^2}{\partial\gamma\partial\Delta}\left[\frac{2}{2\gamma+\Delta}(T_1 + T_2\Delta + T_3\Delta^2 + \cdots)\right] \tag{11}$$

where $\gamma \neq 0$. This expression is non-singular and analytical calculations of the two derivatives in Eq. (11) does not present any problem. The derivation of explicit formulas for the T_1, T_2, T_3, and other coefficients of the Taylor expansion of the $L_p^{(\alpha)}(f; \alpha+\gamma+\Delta)$ function is the last step of this procedure which is much simpler than an alternative method described at the beginning of this Section. Bearing this in mind, below we discuss analytical derivation of explicit formulas for the $I(\alpha, \beta, \gamma; f)$, $J(\alpha, \beta, \gamma; f)$, $I(\alpha, \gamma+\Delta, \gamma; f)$ and $J(\alpha, \gamma+\Delta, \gamma; f)$ integrals.

3 Formulas for the $J(\alpha, \beta, \gamma; f)$ integrals

First, we derive the explicit formulas for the integrals $J(\alpha, \beta, \gamma; f)$ which include the spherical Bessel and Neumann functions. In the case of the spherical Bessel functions

$j_\ell(x)$ which are traditionally defined by the equation

$$j_\ell(x) = \sqrt{\frac{2}{\pi x}} J_{\ell+\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi}} x^{\frac{1}{2}-1} J_{\ell+\frac{1}{2}}(x) \tag{12}$$

the integral $J(\alpha, \beta, \gamma; f)$ is written in the form

$$\begin{aligned} J(\alpha, \beta, \gamma; j_\ell(Vr_{32})) &= \sqrt{\frac{2}{\pi}} \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} r_{32}^{\frac{1}{2}-1} J_{\ell+\frac{1}{2}}(Vr_{32}) \\ &\quad \times \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) dr_{32} dr_{31} dr_{21} \\ &= \sqrt{\frac{2}{\pi}} \frac{2}{\beta^2 - \gamma^2} \Big\{ \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} J_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha+\beta) r_{32}] dr_{32} \\ &\quad - \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} J_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha+\gamma) r_{32}] dr_{32} \Big\} \\ &= \sqrt{\frac{2}{\pi}} \frac{2}{\beta^2 - \gamma^2} \Big[F(\alpha+\beta, V) - F(\alpha+\gamma, V) \Big] \end{aligned} \tag{13}$$

where V is a numerical parameter and the two-argument function F is

$$F(\alpha+\beta, V) = \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} \cdot J_{\ell+\frac{1}{2}}(Vr_{32}) \cdot \exp[-(\alpha+\beta) r_{32}] dr_{32} \tag{14}$$

is the Laplace transform of the $r^{-\frac{1}{2}} \cdot J_{\ell+\frac{1}{2}}(Vr)$ function. By using the formula Eq. (6.621) from [9] we transform the explicit expression for the $F(\alpha+\beta, V)$ function to the form

$$F(\alpha+\beta, V) = \frac{\left(\frac{V}{2}\right)^{\ell+\frac{1}{2}}}{[(\alpha+\beta)^2 + V^2]^{\frac{\ell+1}{2}}} \cdot \frac{\ell!}{\Gamma(\ell+\frac{3}{2})} \cdot {}_2F_1\Big(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; q^2\Big) \tag{15}$$

where $q = \frac{V}{\sqrt{(\alpha+\beta)^2+V^2}} (\leq 1)$ and $\Gamma(z)$ is the Euler's $\Gamma-$function [10]. Note that the hypergeometric function in Eq. (15) is written in the form ${}_2F_1(a, a; a+a+\frac{1}{2}; y)$. Therefore, with the use of the so-called quadratic transformation we can reduce this hypergeometric function to the associated Legendre function of the first kind $P_\nu^\mu(x)$. The final expression for the $F(\alpha+\beta, V)$ function takes the form

$$F(\alpha+\beta, V) = \frac{\ell!}{[(\alpha+\beta)^2 + V^2]^{\frac{1}{4}}} \cdot P_{-\frac{1}{2}}^{-\ell-\frac{1}{2}}\Big(\frac{\alpha+\beta}{\sqrt{[(\alpha+\beta)^2 + V^2]}}\Big) \tag{16}$$

Analogous formulas can be produced for the spherical Bessel functions of the second kind (or Neumann functions) which are defined by the equation

$$n_\ell(x) = \sqrt{\frac{2}{\pi x}} N_{\ell+\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi}} x^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(x) \tag{17}$$

The corresponding three-body integral $I(\alpha, \beta, \gamma; n_\ell(Vr_{32}))$ is written in the form

$$\begin{aligned} I(\alpha, \beta, \gamma; n_\ell(Vr_{32})) &= \sqrt{\frac{2}{\pi}} \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} r_{32}^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(Vr_{32}) \\ &\quad \times \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) \times dr_{32} dr_{31} dr_{21} \\ &= \sqrt{\frac{2}{\pi}} \frac{2}{\beta^2 - \gamma^2} \Big\{ \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha+\beta) r_{32}] dr_{32} \\ &\quad - \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha+\gamma) r_{32}] dr_{32} \Big\} \\ &= \sqrt{\frac{2}{\pi}} \frac{2}{\beta^2 - \gamma^2} \Big[G(\alpha+\beta, V) - G(\alpha+\gamma, V) \Big] \end{aligned} \tag{18}$$

where the G-function is

$$\begin{aligned} G(\alpha+\beta, V) &= \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha+\beta) r_{32}] dr_{32} \\ &= -\frac{2}{\pi} \frac{\ell!}{[(\alpha+\beta)^2 + V^2]^{\frac{1}{4}}} \cdot Q_{-\frac{1}{2}}^{-\ell-\frac{1}{2}} \left(\frac{\alpha+\beta}{\sqrt{[(\alpha+\beta)^2 + V^2]}} \right) \end{aligned} \tag{19}$$

where Q_ν^μ are the associated Legendre functions of the second kind. The explicit expression of the $G(\alpha+\beta, V)$ function written in terms of the hypergeometric functions is extremely cumbersome (see, e.g., the formula at p. 733 in [9]) and is not presented here.

4 Formulas for the partial derivatives

As we mentioned above the formulas presented above for the $J(\alpha, \beta, \gamma; j_\ell(Vr_{32}))$ integrals are not the final formulas which can directly be used in calculations. In actual calculations one needs to determine the third order derivatives from these integrals with respect to the three parameters α, β, γ [see Eq. (5)]. Only after this procedure do we find the values which are the final expressions for three-body integrals arising in actual applications. Analytical computation of the partial derivative of the $J(\alpha, \beta, \gamma; j_\ell(Vr_{32}))$ integrals with respect to the parameter α is straightforward. To produce the explicit formulas for such derivatives note that Eq. (15) can also be written in the form

$$\begin{aligned} F(\alpha+\beta, V) &= \frac{\ell!}{2^\ell \sqrt{2V} \Gamma(\ell+\frac{3}{2})} \cdot (q^2)^{\frac{\ell+1}{2}} \cdot {}_2F_1\left(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; q^2 \right) \\ &= A(\ell, V) \cdot (q^2)^{\frac{\ell+1}{2}} \cdot {}_2F_1\left(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; q^2 \right) \end{aligned} \tag{20}$$

where $q^2 = \frac{V^2}{(\alpha+\beta)^2+V^2}$ and $A(\ell, V) = \frac{\ell!}{2^\ell\sqrt{2V}\Gamma(\ell+\frac{3}{2})}$ is a q-independent function. The partial derivative with respect to the parameter α is determined with the use of the following relation

$$\frac{\partial f}{\partial \alpha} = \frac{2q^4}{V^2}(\alpha+\beta)\frac{\partial f}{\partial q^2} = \frac{\partial f}{\partial \beta} \tag{21}$$

where the function $f = f(\alpha+\beta)$ depends upon the sum $\alpha+\beta$. Analogously, for any function which depends upon the $\alpha+\gamma$ sum the partial derivative is

$$\frac{\partial f_1}{\partial \alpha} = \frac{2q^4}{V^2}(\alpha+\gamma)\frac{\partial f_1}{\partial q^2} = \frac{\partial f_1}{\partial \gamma} \tag{22}$$

where the function f_1 is of the form $f_1 = f_1(\alpha+\gamma)$.

Let us apply these formulas to the $F(\alpha+\beta, V)$ function defined in Eq. (20). For the partial derivative of the $F(\alpha+\beta, V)$ function with respect to α one finds

$$\begin{aligned}\frac{\partial F}{\partial \alpha} &= \frac{(\alpha+\beta)}{V^2}A(\ell, V)(\ell+1)\Big\{(q^2)^{\frac{\ell+7}{2}}\cdot {}_2F_1\Big(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; q^2\Big)\\ &\quad + (q^2)^{\frac{\ell+9}{2}}\cdot\frac{(\ell+1)}{(2\ell+3)}\cdot {}_2F_1\Big(\frac{\ell+3}{2}, \frac{\ell+3}{2}; \ell+\frac{5}{2}; q^2\Big)\Big\} = \frac{\partial F}{\partial \beta}\end{aligned} \tag{23}$$

where we have used the formula

$$\frac{d[{}_2F_1(a, b; c; z)]}{dz} = \frac{ab}{c}\cdot {}_2F_1(a+1, b+1; c+1; z) \tag{24}$$

known from the theory of hypergeometric functions (see, e.g., [10]). These formulas allow one to determine the explicit expression for the following second-order partial derivative

$$\begin{aligned}\frac{\partial^2 F}{\partial \alpha \partial \beta} &= \frac{A(\ell, V)(\ell+1)}{V^2}\Big\{(q^2)^{\frac{\ell+7}{2}}\cdot {}_2F_1\Big(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; q^2\Big)\\ &\quad + (q^2)^{\frac{\ell+9}{2}}\cdot\frac{(\ell+1)}{(2\ell+3)}{}_2F_1\Big(\frac{\ell+3}{2}, \frac{\ell+3}{2}; \ell+\frac{5}{2}; q^2\Big)\Big\} + T_2^{(\beta)}\end{aligned} \tag{25}$$

where the term $T_2^{(\beta)}$ is

$$T_2^{(\beta)} = \frac{2(\alpha+\beta)^2}{V^4}A(\ell, V)(\ell+1)\Big\{q^4\frac{\partial}{\partial q^2}\Big[(q^2)^{\frac{\ell+7}{2}}\cdot {}_2F_1\Big(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; q^2\Big)\Big] \tag{26}$$

$$+\frac{(\ell+1)}{(2\ell+3)}q^4\frac{\partial}{\partial q^2}\Big[(q^2)^{\frac{\ell+9}{2}}{}_2F_1\Big(\frac{\ell+3}{2}, \frac{\ell+3}{2}; \ell+\frac{5}{2}; q^2\Big)\Big]\Big\} \tag{27}$$

The analogous formula for the $F(\alpha + \gamma, V)$ function takes the form

$$\frac{\partial F}{\partial \alpha} = \frac{(\alpha+\gamma)}{V^2} A(\ell, V)(\ell+1)\Big\{(p^2)^{\frac{\ell+7}{2}} \cdot {}_2F_1\Big(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; p^2\Big) + (p^2)^{\frac{\ell+9}{2}} \cdot \frac{(\ell+1)}{2(2\ell+3)} {}_2F_1\Big(\frac{\ell+3}{2}, \frac{\ell+3}{2}; \ell+\frac{5}{2}; p^2\Big)\Big\} = \frac{\partial F}{\partial \gamma} \tag{28}$$

where $p^2 = \frac{V^2}{(\alpha+\gamma)^2+V^2}$. Note that the partial derivative of the functions $F(\alpha + \beta, V)$ and $F(\alpha + \gamma, V)$, Eq. (20), with respect to the parameters α, β and/or γ is always written in the form of a product of the power-type function of q^2 (or p^2) and the hypergeometric function ${}_2F_1$ which also depends upon the variable q^2 (or p^2). This simplifies analytical (and numerical) computation of the three-particle integrals with spherical Bessel and Neumann functions. The second order derivative $\frac{\partial^2 F}{\partial\alpha\partial\gamma}$ equals

$$\frac{\partial^2 F}{\partial\alpha\partial\gamma} = \frac{A(\ell, V)(\ell+1)}{V^2}\Big\{(q^2)^{\frac{\ell+7}{2}} \cdot {}_2F_1\Big(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; q^2\Big) + (q^2)^{\frac{\ell+9}{2}} \cdot \frac{(\ell+1)}{(2\ell+3)} {}_2F_1\Big(\frac{\ell+3}{2}, \frac{\ell+3}{2}; \ell+\frac{5}{2}; q^2\Big)\Big\} + T_2^{(\gamma)} \tag{29}$$

where the term $T_2^{(\gamma)}$ is

$$T_2^{(\gamma)} = \frac{2(\alpha+\gamma)^2}{V^4} A(\ell, V)(\ell+1)\Big\{q^4 \frac{\partial}{\partial q^2}\Big[(q^2)^{\frac{\ell+7}{2}} \cdot {}_2F_1\Big(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell+\frac{3}{2}; q^2\Big)\Big] \tag{30}$$

$$+ \frac{(\ell+1)}{(2\ell+3)} q^4 \frac{\partial}{\partial q^2}\Big[(q^2)^{\frac{\ell+9}{2}} {}_2F_1\Big(\frac{\ell+3}{2}, \frac{\ell+3}{2}; \ell+\frac{5}{2}; q^2\Big)\Big]\Big\} \tag{31}$$

The formulas for the second order derivatives derived above formally solve the problem of analytical calculations of the integral, Eq. (5), since the $F(\alpha + \beta, V)$ function does not depend upon the parameter γ, while the analogous function $F(\alpha + \gamma, V)$ does not depend upon the parameter β. These parameters can be found only in the denominators of the integral $J(\alpha, \beta, \gamma; f)$ defined by Eq. (7). This simplifes all actual calculations of the partial derivatives upon the third non-linear parameter. However, there is a special case when $\beta \approx \gamma$ which corresponds to the exact singularity $\beta = \gamma$ in the formula, Eq. (7). In such cases to determine all required integrals we need to introduce a small parameter $\Delta = \beta - \gamma$ and expand the incident integral $J(\alpha, \beta, \gamma; f) = J(\alpha, \gamma, \Delta; f)$ as a power series written in terms of Δ. Then we need to consider only a few first terms in these series assuming that the parameter Δ is very small and $\gamma \neq 0$.

5 Approach based on the power series expansions of Bessel and Neumann functions

Another aproach widely used to determine three-particle integrals containing spherical Bessel and Neumann functions is based on the use of power series expansions for these functions. In reality, one finds a few different power series expansions for the spherical Bessel and Neumann functions, e.g., expansions which follow from the well known expressions of these functions in terms of some elementary functions. In various applications such expressions often contain trigonometric functions. In particular, the power series expansions based on trigonometric functions ($sinx$ and $cosx$) were used in our earlier paper [6]. Below, we develop a different approach which follows from the 'natural' power series expansion of the spherical Bessel and Neumann functions, e.g., in the case of spherical Bessel functions

$$j_L(z) = z^L \cdot \Big(1 - \frac{z^2}{1! \cdot 2 \cdot (2L+3)} + \frac{z^4}{2! \cdot 2^2 \cdot (2L+3)(2L+5)} - \frac{z^6}{3! \cdot 2^3 \cdot (2L+3)(2L+5)(2L+7)} + \cdots + (-1)^n \frac{z^{2n}}{n! \cdot 2^n \cdot (2L+3)(2L+5) \cdot \ldots \cdot (2L+2n+1)} \qquad (32)$$

Now, we can assume that in this equation $z = pr_{32}$, where p is a real, positive number, and re-write the right-hand side of this equation to the following form

$$j_L(z) = b_{(0;L)} p^L r_{32}^L - b_{(1;L)} p^{L+2} r_{32}^{L+2} + b_{(2;L)} p^{L+4} r_{32}^{L+4} - b_{(3;L)} p^{L+6} r_{32}^{L+6} + \cdots + (-1)^n b_{(3;L)} p^{L+2n} r_{32}^{L+2n} + \ldots \qquad (33)$$

where $b_{(0;L)} = 1$, $b_{(1;L)} = -\frac{1}{2(2L+3)}$ and $b_{(k;L)} = (-1)^k \frac{1}{k!2^k(2L+3)\cdots\cdots(2L+2k+1)}$.

With the help of this expression one finds the following formula for the three-particle integral $\mathcal{J}_L(\alpha, \beta, \gamma; n_1, n_2, n_3)$, Eq. (2), with the Bessel function $j_L(r_{32})$

$$\begin{aligned} &\mathcal{J}_L(\alpha, \beta, \gamma; n_1, n_2, n_3;\ p) \\ &\quad = b_{(0;L)} p^L \Gamma_{L+1,1,1}(\alpha, \beta, \gamma) - b_{(1;L)} p^{L+2} \Gamma_{L+3,1,1}(\alpha, \beta, \gamma) \\ &\qquad + b_{(2;L)} p^{L+4} \Gamma_{L+5,1,1}(\alpha, \beta, \gamma) \\ &\qquad + (-1)^n b_{(n;L)} p^{L+2n} \Gamma_{L+2n+1,1,1}(\alpha, \beta, \gamma) + \cdots \end{aligned} \qquad (34)$$

where the notation $\Gamma_{k,l,n}(\alpha, \beta, \gamma)$ designates the following auxiliary three-body integral

$$\Gamma_{k,l,n}(\alpha, \beta, \gamma) = \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{31}-r_{32}|}^{r_{31}+r_{32}} r_{32}^k r_{31}^l r_{21}^n \times \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) dr_{32} dr_{31} dr_{21} \qquad (35)$$

where $k \geq 0, l \geq 0, n \geq 0$ and $\alpha + \beta > 0, \alpha + \gamma > 0$ and $\beta + \gamma > 0$ (see below). Analytical computation of this integral has extensively been explained in a number of earlier studies. Correspondingly, below we restrict ourselves only to a few following remarks. In perimetric coordinates the integral, Eq. (35), takes the form

$$\Gamma_{k,l,n}(\alpha,\beta,\gamma) = 2\int_0^{\infty}\int_0^{\infty}\int_0^{\infty} exp\Big[-(\alpha+\beta)u_3 - (\alpha+\gamma)u_2 - (\beta+\gamma)u_1\Big] \times (u_2+u_3)^k (u_1+u_3)^l (u_1+u_2)^n du_1 du_2 du_3 \quad (36)$$

where we took into account the fact that the Jacobian of transformation from the relative $(r_{32}, r_{31}.r_{21})$ to perimetric coordinates (u_1, u_2, u_3) equals 2. The integration over three independent perimetric coordinates u_i $(0 \leq u_i < \infty)$ in Eq. (36) is simple and the explicit formula for the $\Gamma_{n,k,l}(\alpha,\beta,\gamma)$ integral is reduced to the form

$$\Gamma_{k;l;n}(\alpha,\beta,\gamma) = 2\sum_{k_1=0}^{k}\sum_{l_1=0}^{l}\sum_{n_1=0}^{n} C_k^{k_1} C_l^{l_1} C_n^{n_1} \times \frac{(l-l_1+k_1)!}{(\alpha+\beta)^{l-l_1+k_1+1}} \frac{(k-k_1+n_1)!}{(\alpha+\gamma)^{k-k_1+n_1+1}} \frac{(n-n_1+l_1)!}{(\beta+\gamma)^{n-n_1+l_1+1}} = 2\cdot k!\cdot l!\cdot n! \times \sum_{k_1=0}^{k}\sum_{l_1=0}^{l}\sum_{n_1=0}^{n} \frac{C_{n-n_1+k_1}^{k_1} C_{k-k_1+l_1}^{l_1} C_{l-l_1+n_1}^{n_1}}{(\alpha+\beta)^{l-l_1+k_1+1}(\alpha+\gamma)^{k-k_1+n_1+1}(\beta+\gamma)^{n-n_1+l_1+1}} \quad (37)$$

where C_k^m are the binomial coefficients (= number of combinations from k by m) (see, e.g., [9]).

Our computational results for some three-particle integrals with the Bessel functions $j_L(pr_{32})$ can be found in Table 1, where a significant attention is given to the three-particle integrals which are important in calculations of the photodetachment cross-section of negeatively charged hydrogen ions. This means $n_1 = 1, n_2 = 1, n_3 = 1$, $L = 1$ (or 0), $p \leq 0.25$, etc. Some other integrals with $L = 2$ and 3 are also shown in Table 1. Tables 2 and 3 contain the photodetachment cross-section of the $^{\infty}H^-$ ion determined for a number of different values of $p = p_e$ (momentum of the outgoing photoelectron). All details of our calculations can be found in [5]. To determine the photodetachment cross-sections given in Tables 2 and 3 we used four approximate eigenfunctions of the ground 1^1S-state of the $^{\infty}H^-$ ion which contain 100, 200, 300 and 350 basis exponential functions in the relative coordinates r_{32}, r_{31}, r_{21} (see discussion in [5]). Numerical highly accurate computations of the three-particle integrals $\mathcal{J}_1(\alpha,\beta,\gamma;1,1,1;p)$ with the spherical Bessel $j_1(pr_{32})$ function plays a cenral role during these calculations. Accurate and complete evaluation of the photodetachment cross-section of negeatively charged hydrogen ions is a paramount importance for prediction of the opacity of Solar photosphere for infrared and visible radiation and for accurate calculations of the thermal balance at our planet. Absorption of radiation by the negatively charged hydrogen ions also plays a crucial role in the photospheres of the late A-stars, F, G and K stars (for more details, see, e.g., [5] and [11–14]).

Table 1 Numerical values of the $\mathcal{J}_L(\alpha, \beta, \gamma; n_1, n_2, n_3)$ integrals which contain the spherical Bessel function $j_L(pr_{32})$, Eq. (2), computed for different values of the $\alpha, \beta, \gamma, n_1, n_2, n_3$ and L, p parameters

α	β	γ	n_1	n_2	n_3	p	L	$\mathcal{J}_L$
1.4640869884366499	0.75420033339371047	−0.026861753412472252	1	1	1	0.005	0	0.67328089814020617E+01
1.0168713023739615	0.24029892072746007	1.6984993699723810	1	1	1	0.005	0	0.72393687894750349E+00
1.4565595733540032	0.28036063969944930	1.9095943716950105	1	1	1	0.005	0	0.18775779926215179E+00
1.1679994723882926	0.63043971281376273	−0.35287359542319671	1	1	1	0.05	1	0.17154004724016701E+02
1.9581235768179751	2.0944368148809208	0.56068822392359250	1	1	1	0.05	1	0.86345114202773180E−03
0.96737010460798024	0.34527545254103408	1.0860811726527724	1	1	1	0.05	1	0.81987782052331701E−01
1.0493783174344522	0.40808546445055934	−0.073333256323020148	1	1	1	0.095	2	0.40124151338323356E+01
−0.36154669521476098	1.0832506365182395	0.69088502941206780	1	1	1	0.095	2	0.57681558596299951E+02
2.5114063922049480	0.84684230034986108	1.8344555246475086	1	1	1	0.095	2	0.46198558565508952E−04
0.23231802441004900	1.7524355357267239	0.54352066894629194	1	1	1	0.125	3	0.11561661833057003E+00
1.7107325146429595	1.0713577531055895	−0.060501061193240962	1	1	1	0.125	3	0.56894681582571403E−02
1.1679994723882926	0.63043971281376273	−0.35287359542319671	1	1	1	0.125	3	0.67135004066637548E+01[a]
1.1679994723882926	0.63043971281376273	−0.35287359542319671	1	1	1	0.125	3	0.67135004066637548E+01[b]
0.19065034447949089	1.6660758235699048	0.54732208390234915	3	2	1	0.150	1	0.55784361764547460E+02
1.7313585008393913	1.0069952364710282	−0.051734066116653426	1	2	3	0.150	2	0.34192450685349652E+01
0.19065034447949089	1.6660758235699048	0.54732208390234915	3	2	2	0.150	0	0.87426327539573991E+03
1.1679994723882926	0.63043971281376273	−0.35287359542319671	2	3	1	0.150	1	0.28308343140217782E+05

[a] For $n_{max} = 20$ in Eq. (34)
[b] For $n_{max} = 40$ in Eq. (34)

Table 2 Photodetachment cross-section (in cm^2) of the negatively charged $^{\infty}H^-$ ion in the ground 1^1S-state

E_{H^-} E_e	-0.5277751016514754 $\sigma(E_e)(N = 100)$	-0.527751016542222 $\sigma(E_e)(N = 200)$	-0.527751016544153 $\sigma(E_e)(N = 300)$	-0.527751016544252 $\sigma(E_e)(N = 350)$
0.0000125	0.2959871598958E−17	0.2959708037311E−17	0.2959861281153E−17	0.2959854603169E−17
0.0001125	0.8795380828880E−17	0.8794948110002E−17	0.8795361962978E−17	0.8795347268968E−17
0.0003125	0.1438360342346E−16	0.1438300909140E−16	0.1438357679058E−16	0.1438356148152E−16
0.0006125	0.1957712288314E−16	0.1957643735991E−16	0.1957704797715E−16	0.1957703477352E−16
0.0010125	0.2425265400821E−16	0.2425191522736E−16	0.2425248779858E−16	0.2425247518253E−16
0.0015125	0.2831698270472E−16	0.2831623914269E−16	0.2831673151310E−16	0.2831671287514E−16
0.0021125	0.3170992749076E−16	0.3170925200030E−16	0.3170965737411E−16	0.3170962354548E−16
0.0028125	0.3440433821549E−16	0.3440381135063E−16	0.3440414647798E−16	0.3440409146283E−16
0.0036125	0.3640352920358E−16	0.3640321523910E−16	0.3640350418486E−16	0.3640342883386E−16
0.0045125	0.3773680407675E−16	0.3773673443071E−16	0.3773699512169E−16	0.3773690666895E−16
0.0055125	0.3845384133828E−16	0.3845400935876E−16	0.3845424767129E−16	0.3845415662293E−16
0.0066125	0.3861868492001E−16	0.3861905054026E−16	0.3861926168889E−16	0.3861917835696E−16
0.0078125	0.3830395973976E−16	0.3830446043948E−16	0.3830463436882E−16	0.3830456649096E−16
0.0091125	0.3758575600990E−16	0.3758632013271E−16	0.3758644736645E−16	0.3758639917081E−16
0.0105125	0.3653944056325E−16	0.3653999965077E−16	0.3654007536656E−16	0.3654004777150E−16
0.0120125	0.3523648973934E−16	0.3523698771025E−16	0.3523701334398E−16	0.3523700477057E−16
0.0136125	0.3374231314689E−16	0.3374271143790E−16	0.3374269418098E−16	0.3374270152781E−16
0.0153125	0.3211495539132E−16	0.3211523424157E−16	0.3211518525441E−16	0.3211520475640E−16
0.0171125	0.3040451970212E−16	0.3040467643263E−16	0.3040460861272E−16	0.3040463646812E−16
0.0190125	0.2865314494953E−16	0.2865319035850E−16	0.2865311628737E−16	0.2865314904517E−16
0.0210125	0.2689537619430E−16	0.2689533014968E−16	0.2689526056870E−16	0.2689529532263E−16
0.0231125	0.2515878988382E−16	0.2515867697255E−16	0.2515861990078E−16	0.2515865435015E−16
0.0253125	0.2346476115434E−16	0.2346460695703E−16	0.2346456740216E−16	0.2346459983308E−16

Table 2 continued

E_{H^-} E_e	−0.5277751016514754 $\sigma(E_e)(N = 100)$	−0.527751016542222 $\sigma(E_e)(N = 200)$	−0.527751016544153 $\sigma(E_e)(N = 300)$	−0.527751016544252 $\sigma(E_e)(N = 350)$
0.0276125	0.2182928758418E−16	0.2182911586458E−16	0.2182909599163E−16	0.2182912521773E−16
0.0300125	0.2026380822337E−16	0.2026363909882E−16	0.2026363869442E−16	0.2026366398150E−16
0.0325125	0.1877597733842E−16	0.1877582634515E−16	0.1877584342631E−16	0.1877586441441E−16
0.0351125	0.1737036862527E−16	0.1737024650783E−16	0.1737027795553E−16	0.1737029458465E−16
0.0378125	0.1604909786307E−16	0.1604901088645E−16	0.1604905302160E−16	0.1604906546358E−16
0.0406125	0.1481236064572E−16	0.1481231123527E−16	0.1481236028999E−16	0.1481236888700E−16
0.0435125	0.1365888760028E−16	0.1365887514331E−16	0.1365892760874E−16	0.1365893281871E−16

N is the total number of basis function in the trial wave function and E is the total energy (in $a.u.$) for this wave function. The final hydrogen atom is formed in the ground 1-state. The notation E_e stands for the energy of the emitted photo-electron (in $a.u.$)

Table 3 Photodetachment cross-section (in cm^2) of the negatively charged $^{\infty}H^-$ ion in the ground 1^1S-state for intermediate energies of photo-electron E_e

E_e	$\sigma(E_e)(N=100)$	$\sigma(E_e)(N=200)$	$\sigma(E_e)(N=300)$	$\sigma(E_e)(N=350)$
0.0465125	0.1258632304494E−16	0.1258634472580E−16	0.1258639757846E−16	0.1258639992733E−16
0.0496125	0.1159153494352E−16	0.1159158652358E−16	0.1159163734473E−16	0.1159163738578E−16
0.0528125	0.1067086476953E−16	0.1067094125823E−16	0.1067098826764E−16	0.1067098654801E−16
0.0561125	0.9820325885784E−17	0.9820422077633E−17	0.9820464104618E−17	0.9820461139031E−17
0.0595125	0.9035758565506E−17	0.9035869438582E−17	0.9035905851910E−17	0.9035902103435E−17
0.0630125	0.8312949036516E−17	0.8313070022232E−17	0.8313100637491E−17	0.8313096504894E−17
0.0666125	0.7647719067068E−17	0.7647846209056E−17	0.7647871188006E−17	0.7647866999040E−17
0.0703125	0.7035991724973E−17	0.7036121748649E−17	0.7036141501167E−17	0.7036137510947E−17
0.0741125	0.6473838090902E−17	0.6473968405712E−17	0.6473983501310E−17	0.6473979894812E−17
0.0780125	0.5957508925751E−17	0.5957637580462E−17	0.5957648673312E−17	0.5957645571010E−17
0.0820125	0.5483454597018E−17	0.5483580205597E−17	0.5483587974654E−17	0.5483585440313E−17
0.0861125	0.5048335965040E−17	0.5048457617334E−17	0.5048462721451E−17	0.5048460771207E−17
0.0903125	0.4649028414276E−17	0.4649145582341E−17	0.4649148629125E−17	0.4649147241080E−17
0.0946125	0.4282620780980E−17	0.4282733228822E−17	0.4282734755358E−17	0.4282733879064E−17
0.0990125	0.3946410568182E−17	0.3946518269998E−17	0.3946518733255E−17	0.3946518298616E−17
0.1035125	0.3637896542435E−17	0.3637999612243E−17	0.3637999386976E−17	0.3637999312224E−17
0.1081125	0.3354769565193E−17	0.3354868199110E−17	0.3354867581199E−17	0.3354867779736E−17
0.1128125	0.3094902316515E−17	0.3094996747651E−17	0.3094995961090E−17	0.3094996347097E−17
0.1176125	0.2856338412157E−17	0.2856428877305E−17	0.2856428083343E−17	0.2856428576147E−17
0.1225125	0.2637281290488E−17	0.2637368007250E−17	0.2637367314499E−17	0.2637367841750E−17
0.1275125	0.2436083147089E−17	0.2436166299831E−17	0.2436165774447E−17	0.2436166274218E−17
0.1326125	0.2251234117600E−17	0.2251313850531E−17	0.2251313525848E−17	0.2251313947789E−17
0.1378125	0.2081351849141E−17	0.2081428264891E−17	0.2081428150094E−17	0.2081428455791E−17

Table 3 continued

E_e	$\sigma(E_e)(N = 100)$	$\sigma(E_e)(N = 200)$	$\sigma(E_e)(N = 300)$	$\sigma(E_e)(N = 350)$
0.1431125	0.1925171554171E−17	0.1925244716369E−17	0.1925244803977E−17	0.1925244966678E−17
0.1485125	0.1781536605105E−17	0.1781606543651E−17	0.1781606815719E−17	0.1781606819574E−17
0.1540125	0.1649389701120E−17	0.1649456419055E−17	0.1649456852113E−17	0.1649456691077E−17
0.1596125	0.1527764618567E−17	0.1527828099671E−17	0.1527828668478E−17	0.1527828344977E−17
0.1653125	0.1415778541692E−17	0.1415838758120E−17	0.1415839438357E−17	0.1415838961857E−17
0.1711125	0.1312624959855E−17	0.1312681879323E−17	0.1312682649388E−17	0.1312682034922E−17
0.1770125	0.1217567110132E−17	0.1217620702320E−17	0.1217621544363E−17	0.1217620811106E−17

All notations are the same as in the previous Table

We have represented the unknown integral $\mathcal{J}_L(\alpha, \beta, \gamma; n_1, n_2, n_3; p)$ in the form of a sum of some special auxiliary three-body integrals $\Gamma_{L+2m,1,1}(\alpha, \beta, \gamma)$ for $m = 0, 1, 2, \ldots$. Analytical and numerical calculations of the three-particle integrals which include the corresponding Neumann functions $n_L(pr_{32})$ are significantly more difficult, since some of the (first) three-particle auxiliary integrals $\Gamma_{-k,1,1}(\alpha, \beta, \gamma)$ arising during this process and included in the expansion similar to Eq. (34) are singular. Each singular integral contains a few singular terms which depend upon the cut-off parameter ϵ as $\ln \epsilon + \gamma_E$, $\frac{1}{\epsilon}$, $\frac{1}{\epsilon^2}$, $\frac{1}{\epsilon^3}$, etc, where $\gamma_E = 0.577215\,664901\,53286\ldots$ is the Euler constant. The general structure of these integrals can be understood from the explicit expressions for some of them

$$\Gamma_{-1;1;1}(\alpha, \beta, \gamma) = -\frac{16\beta\gamma[\ln(\alpha+\beta) - \ln(\alpha+\gamma)]}{(\beta^3-\gamma^2)^3} + \frac{4}{(\beta^2-\gamma^2)^2}\Big[\frac{\beta}{\alpha+\gamma} + \frac{\gamma}{\alpha+\beta}\Big] \tag{38}$$

$$\Gamma_{-2;1;1}(\alpha, \beta, \gamma) = -4\frac{\ln\epsilon - \psi(1)}{(\beta+\gamma)^3} + \frac{4}{(\beta^2-\gamma^2)}[(4\alpha\beta\gamma + 3\beta^2\gamma + \gamma^3)\ln(\alpha+\beta) - (4\alpha\beta\gamma + 3\beta\gamma^2 + \beta^3)\ln(\alpha+\gamma)] - \frac{16\beta\gamma}{(\beta+\gamma)^3(\beta-\gamma)^2} \tag{39}$$

$$\Gamma_{-3;1;1}(\alpha, \beta, \gamma) = \frac{4}{\epsilon(\beta+\gamma)^3} + \frac{4\alpha(\ln\epsilon - \psi(2))}{(\beta+\gamma)^3} + \frac{4\beta\gamma(2\alpha+\beta+\gamma)}{(\beta+\gamma)^3(\beta-\gamma)^2} + \frac{4\ln(\alpha+\gamma)[\alpha\beta(3\gamma^2+\beta^2) + \beta\gamma(2\alpha^2+\beta^2+\gamma^2)}{(\beta^2-\gamma^2)^3} - \frac{4\ln(\alpha+\beta)[\alpha\gamma(3\beta^2+\gamma^2) + \beta\gamma(2\alpha^2+\beta^2+\gamma^2)}{(\beta^2-\gamma^2)^3} \tag{40}$$

where $\psi(n)$ is the is the psi-function (or ψ function) [9] (see pp. 952–956). For positive integer n the psi−function is: $\psi(n) = -\gamma_E + \sum_{k=1}^{n-1}\frac{1}{k}$ and γ_E is the Euler constant (see above).

It is clear the auxiliary integral $\Gamma_{-1;1;1}(\alpha, \beta, \gamma)$ is not singular, while the integrals $\Gamma_{-2;1;1}(\alpha, \beta, \gamma)$ and $\Gamma_{-3;1;1}(\alpha, \beta, \gamma)$ are singular. Note that all $\Gamma_{-n;1;1}(\alpha, \beta, \gamma)$ integrals with $n \geq 2$ contain the regular part and principal (or singular), ϵ-dependent part. This complicates operations with such integrals.

6 Recursion formula for three-particle integrals

Another approach in the calculation of the three-particle integrals integrals is based on the well known recursion relations [15] for the spherical Bessel and Neumann functions

$$j_{L+1}(z) = \Big(\frac{2L+1}{z}\Big)j_L(z) - j_{L-1}(z) \quad and$$
$$n_{L+1}(z) = \Big(\frac{2L+1}{z}\Big)n_L(z) - n_{L-1}(z) \tag{41}$$

By assuming that $z = r_{32}$ in both equalities and calculating three-particle integrals Eqs. (1) and (2) from both sides of these equations one finds the two following relations:

$$\mathcal{J}_{L+1}(n_1, n_2, n_3) = (2L+1)\mathcal{J}_L(n_1 - 1, n_2, n_3) + \mathcal{J}_{L-1}(n_1, n_2, n_3) \quad (42)$$

and

$$\mathcal{N}_{L+1}(n_1, n_2, n_3) = (2L+1)\mathcal{N}_L(n_1 - 1, n_2, n_3) + \mathcal{N}_{L-1}(n_1, n_2, n_3) \quad (43)$$

for three-particle integrals with the Bessel and Neumann functions, respectively. The equalities Eqs. (42) and (43) allow one to determine the three-particle integrals on the right-hand sides of these equalities, if we know the three-particle integrals from their left-hand sides. In Eqs. (42) and (43) we apply the following short notations which are simply related with the corresponding notations from in Eqs. (1) and (2): $\mathcal{J}_L(n_1, n_2, n_3) = \mathcal{J}_L(\alpha, \beta, \gamma; n_1, n_2, n_3)$ and $\mathcal{N}_L(n_1, n_2, n_3) = \mathcal{N}_L(\alpha, \beta, \gamma; n_1, n_2, n_3)$. The approach based on the use of recursion formulas for the Bessel and Neumann functions is an effective way to compute a large number of three-particle integrals with different powers of the relative coordinates (n_1, n_2 and n_3). It is important to note that this approach does not lead to any loss of numerical accuracy.

7 Conclusion

We have developed a few different approaches which can sucessufully be used in calculations of three-particles integrals containing spherical Bessel functions of the first and second kind (or Bessel and Neumann functions, respectively). One of these methods is based on the use of the general analytical formula, Eqs. (6)–(7), derived for three-particle integrals written in the relative coordinates r_{32}, r_{31} and r_{21}. In actual applications this new approach has a number of obvious advantages. Another approach is based on the use of power series expansions for the Bessel and Neumann functions. Based on our experience in evaluating three-particle integrals containing spherical Bessel functions of the first and second kind in any application, it is important to use a few different approaches to determine such integrals and compare final results in terms of numerical stability and overall accuracy.

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