Collective multipole expansions and the perturbation theory in the quantum three-body problem

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Abstract

The perturbation theory with respect to the potential energy of three particles is considered. The first-order correction to the continuum wave function of three free particles is derived. It is shown that the use of the collective multipole expansion of the free three-body Green function over the set of Wigner D-functions can reduce the dimensionality of perturbative matrix elements from twelve to six. The explicit expressions for the coefficients of the collective multipole expansion of the free Green function are derived. It is found that the S-wave multipole coefficient depends only upon three variables instead of six as higher multipoles do. The possible applications of the developed theory to the three-body molecular break-up processes are discussed.

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I. INTRODUCTION

The study of angular distributions in processes of three-particle fragmentation is an important source of information about the dynamics of many physical objects such as atoms and molecules.

Till recently, the experimental technique allowed one to analyze the angular distributions only for charged particles resulting from the many-body fragmentation. In such situations, the structure of the angular distributions is determined by the Coulomb force. For example, this is realized in the process of two-electron single-photon ionization of Helium atom which is quite well studied both experimentally and theoretically [1].

During the last decade, the progress of experimental technique has made it possible to investigate the angular distributions of neutral fragments arising in the processes of three-atomic molecular break-up. Namely, in [2] the dissociative recombination of water ion into the neutral atomic fragments has been studied. In a series of experiments [3, 4, 5] the angular distributions in the predissociation of the triatomic hydrogen into three hydrogen atoms were investigated. Clearly, the analysis of angular distributions in molecular break-up processes could gain significant insight into the nature of chemical forces.

In molecular physics the dynamics of the interacting atoms is usually described within the framework of the Born-Oppenheimer approximation. In this approach the interaction of ions is represented by the set of potential energy surfaces (PES) which are, in fact, the mean field of the electrons. It is important that, generally, PES cannot be decomposed into a sum of binary potentials (i.e. pairwise interactions). Rather, it will contain the terms which “entangle” the coordinates of all particles thus making the standard methods (such as Faddeev approach [6]) inapplicable. Thus, the development of an adequate theory of many-particle molecular fragmentation is a complicated task. Therefore, it is highly desirable to have simple yet physically meaningful models of the molecular break-up.

In the break-up into the neutral fragments often the situation is realized when the kinetic energy of fragments prevails over their interaction potential. This opens the possibility to apply the perturbation theory to the calculation of the wave function of three-particle continuum. In the presented paper the lowest-order perturbation theory with respect to the potential energy was applied to the quantum three-body system. Even in this simplest case the calculation of the matrix elements leads to twelve-dimensional integrals. However, it
turns out that the dimensionality of these integrals can be reduced from twelve to six by employing the technique of collective multipole expansions. This technique was used in [7] where such an expansion was derived for the product of two three-dimensional plane waves \( \exp(i(q_1 \cdot r_1 + q_2 \cdot r_2)) \). Note that the results presented in the paper allows one to simplify the calculation of the matrix elements within the perturbative approximation even if the potential contains three-body (i.e. non-binary) terms.

The paper is organized as follows. In Sec. II the general equations of the perturbation theory are derived. They are based on the expression for the Green function corresponding to a system of three free particles. The calculation of matrix elements involving the perturbative wave functions is considered in Sec. III. In that section it is also demonstrated how the calculations can be simplified by employing the collective multipole expansion of the free Green function over the basis set of Wigner \( D \)-functions. The coefficients of that expansion are calculated in Secs. IV, V using two different approaches. In Sec. IV the expressions for multipole coefficients are derived by calculating the overlap integral of the free Green function with Wigner \( D \)-function. The expansion of the free Green function over the set of six-dimensional hyperspherical harmonics is considered in Sec. V. The derived results are discussed in Sec. VI where some concluding remarks are also given. Appendix A contains details of computations of the integral with the free Green function over the Euler angles. The summary of properties of the set of six-dimensional hyperspherical harmonics labeled by the particle’s individual angular momenta quantum numbers is given in Appendix B.

The convention \( \hbar = 1 \) is used throughout the text. Capital letters denote the six-dimensional vectors, e.g. \( R = (r_1, r_2) \), where \( r_1, r_2 \) are three-dimensional vectors, \( R = |R| = \sqrt{r_1^2 + r_2^2} \).

II. THE GENERAL FORMALISM

We begin by writing the Schroedinger equation for the system of three particles with masses \( m_1, m_2, m_3 \),

\[
\left( -\frac{1}{2\mu_1} \frac{\partial^2}{\partial r_1^2} - \frac{1}{2\mu_2} \frac{\partial^2}{\partial r_2^2} + U - E \right) \Psi(r_1, r_2) = 0. \tag{1}
\]

Here, \( r_1 \) and \( r_2 \) are Jacobi vectors (see fig. I) and the reduced masses \( \mu_1, \mu_2 \) are defined by

\[
\frac{1}{\mu_1} = \frac{1}{m_2} + \frac{1}{m_3}, \quad \frac{1}{\mu_2} = \frac{1}{m_1} + \frac{1}{m_2 + m_3}. \tag{2}
\]
FIG. 1: Jacobi vectors for the three-body system. $CM_{23}$ is the CM of the particles $m_2$ and $m_3$.

It is convenient to replace $r_1 \rightarrow \sqrt{\mu_1} r_1$, $r_2 \rightarrow \sqrt{\mu_2} r_2$ in eq. (1) which thereby becomes

$$\left(\Delta_6 - 2[U - E]\right) \Psi(r_1, r_2) = 0, \quad \Delta_6 = \frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2}. \quad (3)$$

In this equation the potential energy depends on the masses of particles, but the kinetic energy operator does not.

Below the situation is considered when the potential energy of the three-body system is much smaller than the total (non-negative) energy $E$. Introducing the wave number $Q$ of the continuum state by $E = Q^2/2$, we write

$$\left(\Delta_6 - 2U + Q^2\right) \Psi(r_1, r_2) = 0, \quad (4)$$

We approximate the total wave function by the combination $\Psi = \Psi^{(0)} + \Psi^{(1)}$, where $\Psi^{(0)}$ is independent of $U$, and $\Psi^{(1)}$ scales as $\Psi \rightarrow c \Psi$ at $U \rightarrow c U$. Substituting this decomposition into eq. (4) and comparing the coefficients which scale equally, we obtain

$$\left(\Delta_6 + Q^2\right) \Psi^{(0)}(r_1, r_2) = 0,$$
$$\left(\Delta_6 + Q^2\right) \Psi^{(1)}(r_1, r_2) = 2U \Psi^{(0)}. \quad (5)$$

In the zeroth-order approximation the wave function is the product of two three-dimensional plane waves

$$\Psi^{(0)}(r_1, r_2) = e^{i(Q \cdot R)}, \quad (Q \cdot R) = (q_1 \cdot r_1) + (q_2 \cdot r_2), \quad (6)$$

where $q_{1,2}$ are the linear momenta vectors conjugated to the Jacobi vectors $r_{1,2}$. Consequently, the second equation in (5) becomes

$$\left(\Delta_6 + Q^2\right) \Psi^{(1)}(r_1, r_2) = 2U e^{i(Q \cdot R)}. \quad (7)$$

In order to solve this equation we first consider its homogeneous form

$$\left(\Delta_6 + Q^2\right) \Phi(R) = 0. \quad (8)$$
We are interested in a solution depending only on the hyper-radius $R$. Therefore, we have to omit the angular part of the Laplacian $\Delta_6$, which yields

$$\left( \frac{\partial^2}{\partial R^2} + \frac{5}{R} \frac{\partial}{\partial R} + Q^2 \right) \Phi(R) = 0. \tag{9}$$

Introducing the function $F = \Phi/R^2$, this equation transforms to

$$\frac{\partial^2 F}{\partial R^2} + \frac{1}{R} \frac{\partial F}{\partial R} + \left( Q^2 - \frac{4}{R} \right) F(R) = 0. \tag{10}$$

The general solution of this equation is the combination of two Hankel functions $H_2^{(1)}(QR)$ and $H_2^{(2)}(QR) \ [8]$. We note that $H_2^{(1)}(QR)$ at large $R$ has the asymptote of the outgoing spherical wave $[17]

$$H_2^{(1)}(QR) \approx -\left( \frac{2}{\pi QR} \right)^{1/2} e^{i(QR-\pi/4)}, \quad R \to \infty. \tag{11}$$

Thus, the solution of (9) can be chosen to be

$$\Phi(R) = \frac{H_2^{(1)}(QR)}{R^2}. \tag{12}$$

This function satisfies eq. (8) everywhere except $R = 0$. Below we shall prove that

$$G(R) = G(R) = -i \left( \frac{Q}{4\pi R} \right)^2 H_2^{(1)}(QR). \tag{13}$$

is the Green function of the equation (8), that is the solution of the inhomogeneous equation

$$\left( \Delta^{(6)} + Q^2 \right) G(R) = \delta(R). \tag{14}$$

Indeed, at $R > 0$ this function satisfies the homogeneous equation (8). At the limit $R \to 0$ there is a divergency,

$$G(R) \approx -i \left( \frac{Q}{4\pi R} \right)^2 - i \left( \frac{2}{QR} \right)^2 = \frac{-1}{4\pi^3 R^4}. \tag{15}$$

From the properties of Dirac $\delta$-function it follows that integral of (14) taken over the arbitrary region which includes the point $R = 0$ must be equal to unity. We calculate the six-dimensional integral of (14) taken over the infinitesimal sphere $V_\epsilon$ with its center in $R = 0$,

$$\int_{V_\epsilon} \left( \Delta_6 + Q^2 \right) G(R)d^6 R = \int_{S_\epsilon} dS \cdot \nabla_6 G(R) \bigg|_{R=\epsilon} + \pi^3 Q^2 \int_0^\epsilon G(R)R^5 dR. \tag{16}$$
Here, the Gauss theorem has been used in order to transform the volume integral into the integral over the surface of 6-sphere $S_\epsilon$ with the radius $\epsilon$. Noting the expression for the vector surface element $d\mathbf{S} = (\mathbf{R}/R) \epsilon^5 dS$, the integral at $\epsilon \to 0$ evaluates to

$$
\int_{V_\epsilon} \left( \Delta_6 + Q^2 \right) G(R) d^6 R \approx \frac{1}{\pi^3} \int_{S_\epsilon} dS - \frac{Q^2}{4} \int_0^\epsilon R dR = 1 - \frac{\epsilon^2 Q^2}{8} \to 1.
$$

As is seen, $G(R)$ defined by eq. (13) does satisfy the equation (14).

Having Green function (13), the solution of the equation (7) can be immediately written as

$$
\Psi^{(1)}(\mathbf{R}) = 2 \int e^{i(\mathbf{Q} \cdot \mathbf{R}')} U(\mathbf{R}') G(|\mathbf{R} - \mathbf{R}'|) d^6 \mathbf{R}'.
$$

Thus, the continuum wave function $\Psi(\mathbf{R})$ of three particles within the perturbative approach has the form

$$
\Psi(\mathbf{R}) = \Psi_{\mathbf{Q}}(\mathbf{R}) = e^{i\mathbf{Q} \cdot \mathbf{R}} - i \frac{Q^2}{8\pi^2} \int e^{i(\mathbf{Q} \cdot \mathbf{R}')} U(\mathbf{R}') \frac{H_{2}^{(1)}(Q |\mathbf{R} - \mathbf{R}'| \times \mathbf{R} \times \mathbf{R}')}{|\mathbf{R} - \mathbf{R}'|^2} d^6 \mathbf{R}'.
$$

III. THE CALCULATION OF THE MATRIX ELEMENTS WITH THE CORRECTION TERM

In many physical applications it is necessary to calculate the matrix element

$$
M_{j\mu} = \langle \Psi_{j\mu} | \mathcal{O} | \Psi_{\mathbf{Q}} \rangle,
$$

where $\mathcal{O}$ is the transition operator and $\Psi_{j\mu}$ is the wave function which corresponds to the state having the total angular momentum numbers $j\mu$. Without loss of generality, we can assume that $\mathcal{O}$ is a scalar operator. This situation realizes, for example, in the case of the three-atomic molecular predissociation where $\mathcal{O}$ represents the operator of non-adiabatic couplings [5]. If the transition operator is a tensor $\mathcal{O}_{lm}$ then the product $\Psi_{j\mu} \mathcal{O}_{lm}$ can be decomposed into irreducible parts [9] so that the matrix element will be decomposed into the sum of matrix elements of the kind (20).

We note that (20) is the six-dimensional integral,

$$
M_{j\mu} = \int \Psi_{j\mu}^* (\mathbf{R}) \mathcal{O} \Psi_{\mathbf{Q}}(\mathbf{R}) d^6 \mathbf{R}.
$$

Among the six variables three can be chosen to be the collective angles determining the orientation of the whole system in space. The remaining three “shape” variables $\xi$ determine
the internal dynamics of the system and they can be chosen to be \( \xi = r_1, r_2, \cos \theta \), where \( \theta \) is the angle between \( r_1 \) and \( r_2 \). Thus, the transition operator \( \mathcal{O} \) is the function of \( \xi \), \( \mathcal{O} = \mathcal{O}(\xi) \).

Substituting the decomposition (19) into (21) one arrives at the expression

\[
M_{j\mu} = M_{j\mu}^{(0)} + M_{j\mu}^{(1)},
\]

where the zero- and first-order matrix elements are defined by

\[
M_{j\mu}^{(0)} = \int \Psi_{j\mu}^*(\mathbf{R}) \mathcal{O} e^{i(\mathbf{Q} \cdot \mathbf{R})} d^6 R,
\]

\[
M_{j\mu}^{(1)} = -\frac{iQ^2}{8\pi^2} \int \Psi_{j\mu}^*(\mathbf{R}) \mathcal{O} \int e^{i(\mathbf{Q} \cdot \mathbf{R}') U(\xi')} H_2^{(1)}(Q|R' - R|) \frac{H_2^{(1)}(Q|R' - R|)}{|R' - R|^2} d^6 R' d^6 R.
\]

Here, by writing \( U(\xi') \) we make the assumption that the potential energy depends only on the three shape variables. This is true if the three-body system in not a subject of external forces.

The calculation of the matrix element \( M_{j\mu}^{(0)} \) has been considered in [7]. Therefore, below we concentrate on the problem of calculation of the first-order (with respect to the potential) matrix element \( M_{j\mu}^{(1)} \).

As is seen, \( M_{j\mu}^{(1)} \) is determined by the 12-dimensional integral. However, six of twelve variables are the collective angles describing the rotation of the whole system from the coordinate frame defined by Jacobi vectors \( (r_1, r_2) \) to the frame defined by \( (r'_1, r'_2) \) and from the frame \( (r_1, r_2) \) to \( (q_1, q_2) \). Noting that the potential energy does not depend on collective angles, one can try to integrate them out analytically. In order to do so one has to expand the integrands over the basis of angular functions depending on the collective angles. It is convenient to choose as the angular basis the set of Wigner D-functions [9].

The initial state wave function \( \Psi_{j\mu}(\xi) \) can be decomposed into the combination of \((2j+1)\) “internal” wave functions \( \psi_{j\nu}(\xi) \), depending on three shape variables \( \xi \),

\[
\Psi_{j\mu}(\mathbf{R}) = \sum_{\nu=-j}^{j} \psi_{j\nu}(\xi) D_{\nu,\mu}^j(\Omega),
\]

where \( \Omega \) denotes three collective Euler angles describing the rotation from the body-fixed frame (BF) defined by the Jacobi vectors \( \mathbf{R} = (r_1, r_2) \) to the laboratory frame (LF) defined by the momenta vectors \( \mathbf{Q} = (q_1, q_2) \).

At this stage we have to evaluate the angular integral

\[
I_{\mathbf{Q}}(\mathbf{R}) = \int e^{i(\mathbf{Q} \cdot \mathbf{R}')} \frac{H_2^{(1)}(Q|R' - R|)}{|R' - R|^2} d^3 \Omega',
\]

7
where \( \Omega' \) denotes three Euler angles describing the rotation from BF' defined by the pair of Jacobi vectors \( \mathbf{R}' = (r'_1, r'_2) \) to LF.

The calculation of \( I_{\mathbf{Q}}(\mathbf{R}) \) can be performed by taking the multipole expansion of both integrand functions,

\[
e^{i(Q \cdot R')} = \sum_{j=0}^{\infty} \sum_{\mu, \nu} F_{\mu, \nu}^{(j)}(\xi_q; \xi') D_{\mu, \nu}^{(j)}(\Omega'),
\]

\[
\frac{H_2^{(1)}(Q | R' - R |)}{|R' - R|^2} = \sum_{j=0}^{\infty} \frac{2j + 1}{8\pi^2} \sum_{\mu, \nu} G_{\mu, \nu}^{(j)}(\xi; \xi') D_{\mu, \nu}^{(j)}(\Omega''),
\]

where \( \Omega'' \) describes the rotation from BF defined by \( (r_1, r_2) \) to BF' defined by \( (r'_1, r'_2) \). In the upper equation \( \xi_q \) denotes three “shape” variables in the momentum space, e.g. \( \xi_q = q_1, q_2, \cos \chi \), where \( \chi \) is the angle between \( q_1 \) and \( q_2 \).

Note that the rotation \( \Omega'' \) can be presented as a product of rotations

\[
\Omega'' = \Omega \times \Omega'^{-1}.
\]

In terms of Wigner D-functions this equation reads

\[
D_{\mu, \nu}^{(j)}(\Omega'') = \sum_{\nu' = -j}^{j} D_{\mu, \nu}^{(j)}(\Omega) D_{\nu', \nu}^{(j)}(\Omega'^{-1}) = \sum_{\nu' = -j}^{j} D_{\mu, \nu}^{(j)}(\Omega) [D_{\nu', -\nu}^{(j)}(\Omega')^*].
\]

Substituting this equation and eqs. (26) into eq. (25), we arrive at the identity

\[
I_{\mathbf{Q}}(\mathbf{R}) = \sum_{j, j'=0}^{\infty} \frac{2j' + 1}{8\pi^2} \sum_{\mu, \nu, \mu', \nu'} F_{\mu, \nu}^{(j)}(\xi_q; \xi') G_{\mu', \nu'}^{(j)}(\xi; \xi') D_{\mu', \nu'}^{(j)}(\Omega)
\times \int D_{\mu, \nu}^{(j)}(\Omega'') [D_{\nu', -\nu}^{(j)}(\Omega')^*] d\Omega'.
\]

The integration gives \( \delta_{j,j'} \delta_{\mu,-\nu} \delta_{\nu,-\nu'} 8\pi^2/(2j + 1) \) so that

\[
I_{\mathbf{Q}}(\mathbf{R}) = \sum_{j=0}^{\infty} \sum_{\mu, \mu'} F_{\mu', -\nu}(\xi_q, \xi') G_{\mu, -\mu'}(\xi; \xi') D_{\mu, \nu}^{(j)}(\Omega).
\]

Inserting this equation together with eq. (24) for the initial wave function into eq. (23) for the matrix element \( M_{j\mu}^{(1)} \), one can integrate out the angles \( \Omega \). The result is

\[
M_{j\mu}^{(1)} = \frac{-i Q^2}{2j + 1} \sum_{\nu = -j}^{j} \int \psi_{j\nu}^*(\xi) O(\xi) \sum_{\mu' = -j}^{j} \int G_{\nu', -\mu'}^{(j)}(\xi; \xi') F_{\mu', -\mu}(\xi_q, \xi') U(\xi') d^3\xi' d^3\xi.
\]

As is seen, the 12-dimensional integral (23) is reduced to the 6-dimensional integral.
In the next sections we consider the problem of the calculation of the collective multipole coefficients $G_{\mu,\nu}^{(j)}(\xi;\xi')$ introduced in eq. (26). As a preliminary, we note that these coefficients obey the symmetry relation

$$[G_{\mu,\nu}^{(j)}(\xi;\xi')]^* = (-1)^{\mu-\nu} G_{-\mu,-\nu}^{(j)}(\xi;\xi')$$

(32)

which follows from the symmetry property of D-functions $D_{\mu,\nu}(\Omega) = (-1)^{\mu-\nu}[D_{-\mu,-\nu}(\Omega)]^*$. Thus, in practice it is enough to calculate only the coefficients with $\mu \geq \nu$.

For the sake of completeness we present also the expression for the volume element of the shape space for two most often used choices of the set of shape variables $\xi$

$$\int d^3\xi = \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \int_0^{\pi} \sin \theta d\theta = \int_0^\infty R^5 dR \int_0^{\pi/2} \sin^2 2\alpha d\alpha \int_0^{\pi} \sin \theta d\theta,$$

(33)

where the second equation corresponds to the hyperspherical set $\xi = R, \alpha, \theta$, where $R = \sqrt{r_1^2 + r_2^2}$ is the hyperradius and $\alpha = \arctan(r_2/r_1)$ is the hyperangle, so that

$$r_1 = R \cos \alpha, \quad r_2 = R \sin \alpha, \quad 0 \leq \alpha \leq \pi/2.$$  

(34)

IV. MULTIPOLe COEFFICIENTS FOR THE ANGLE-BISECTOR GAUGE

Using the orthogonality of D-functions the expression for the multipole coefficients $G_{\mu,\nu}^{(j)}$ can be written as the three-dimensional integral,

$$G_{\mu,\nu}^{(j)}(\xi;\xi') = \int \frac{H_2^{(1)}(Q|\mathbf{R}' - \mathbf{R}|)}{|\mathbf{R}' - \mathbf{R}|^2} [D_{\mu,\nu}(\Omega'')]^* d^3\Omega''.$$  

(35)

Here, apart of D-functions, Euler angles $\Omega''$ enter the integrand through the term $|\mathbf{R} - \mathbf{R}'|$ which is

$$|\mathbf{R} - \mathbf{R}'| = \sqrt{R^2 + R'^2 - 2p}, \quad p = (\mathbf{r}_1 \cdot \mathbf{r}_1') + (\mathbf{r}_2 \cdot \mathbf{r}_2'),$$

(36)

where only the parameter $p$ depends on $\Omega''$.

At this stage, one has to specify explicitly how the axes of the BF and BF' are connected to the Jacobi vectors $(\mathbf{r}_1, \mathbf{r}_2)$ and $(\mathbf{r}_1', \mathbf{r}_2')$. This procedure is not unique and, therefore, it can be denoted as the “gauge convention” [10].

Below we use angle-bisector gauge for both BF and BF', see fig. 2. Since $p$ is scalar, it does not matter in which frame we calculate it. Let it be BF'. In this frame the components
FIG. 2: The angle-bisector gauge: the $x$-axis is directed along the bisector of the angle between the unit vectors $\hat{r}_1$ and $\hat{r}_2$. The $z$-axis is directed along the vector product $[\hat{r}_1 \times \hat{r}_2]$. $\text{BF}'$ is defined analogously.

The components of $\mathbf{R}'$ have the form

$$
\mathbf{r}'_1 = r'_1 [\cos(\theta'/2), -\sin(\theta'/2), 0],
$$

$$
\mathbf{r}'_2 = r'_2 [\cos(\theta'/2), \sin(\theta'/2), 0],
$$

(37)

The components of $\mathbf{R}$ in $\text{BF}'$ can be calculated using the equation

$$
(\mathbf{r}_n)_i = \sum_{k=x,y,z} (\mathbf{r}_n)_k \mathcal{A}_{ki}(\Omega''), \quad n = 1, 2.
$$

(38)

where $\mathcal{A}_{ki}(\Omega'')$ denotes the components of the rotation matrix [9] and $(\mathbf{r}_n)_k$ is $k$-th component of $\mathbf{r}_n$ in $\text{BF}$ where it is given by eq. (37) with dashes removed. From eq. (38) follows the identity

$$
p = \sum_{i,k} ((\mathbf{r}'_1)_i (\mathbf{r}'_2)_i \mathcal{A}_{ki} + (\mathbf{r}'_2)_i (\mathbf{r}'_1)_i \mathcal{A}_{ki}).
$$

Using explicit form of the rotation matrix $\mathcal{A}$, after some algebraic transformations described in detail in [7], the parameter $p$ can be written as

$$
p = a_1 \sin(\alpha + \gamma + \delta_1) - a_2 \sin(\alpha - \gamma + \delta_2).
$$

(39)

where the parameters are defined by

$$
a_1 = \rho_1 \left( \cos \frac{\beta}{2} \right)^2, \quad a_1 = \rho_2 \left( \sin \frac{\beta}{2} \right)^2,
$$

$$
\rho_{1,2}^2 = (r_1 r'_1)^2 + (r_2 r'_2)^2 + 2 r_1 r_2 r'_1 r'_2 \cos(\theta \mp \theta'),
$$

(40)

where $\rho_1$ corresponds to $(\theta - \theta')$. The additional phases $\delta_{1,2}$ are defined by

$$
\sin \delta_{1,2} = \frac{r_1 r'_1 + r'_2 r_2}{\rho_{1,2}} \cos \frac{\theta \mp \theta'}{2},
$$

$$
\cos \delta_{1,2} = \frac{r_2 r'_2 - r'_1 r_1}{\rho_{1,2}} \sin \frac{\theta \mp \theta'}{2},
$$

(41)
where the upper sign corresponds to $\delta_1$.

In order to calculate the integral in (35) we employ the series expansion (eq. (7.15.18) of [8]),

$$
\frac{H^{(1)}_2(Q|\mathbf{R'} - \mathbf{R}|)}{|\mathbf{R'} - \mathbf{R}|^2} = \sum_{n=0}^{\infty} \frac{(Q p)^n}{n!} \frac{H^{(1)}_{n+2} (Q \sqrt{R^2 + R'^2})}{(R^2 + R'^2)^{n/2}+1}.
$$

(42)

Thus, the expression for the collective multipoles can be written as

$$
G^j_{\mu,\nu}(\xi, \xi') = \sum_{n=0}^{\infty} P^{(j\mu\nu)}_n Q^n \frac{H^{(1)}_{2m+\mu+2} (Q \sqrt{R^2 + R'^2})}{(R^2 + R'^2)^{n/2}+1},
$$

(43)

where the functions $P^{(j\mu\nu)}_n$ are defined by the integral

$$
P^{(j\mu\nu)}_n = \frac{1}{n!} \int p^n [D^{j}_{\mu,\nu} (\Omega'')]^* d^3\Omega''.
$$

(44)

This integral is calculated in Appendix A (see eq. (A10)). In Appendix A it is also demonstrated that the functions $P^{(j\mu\nu)}_n$ are non-zero only for indices $\mu, \nu$ and $n$ having the same parity. Hence, the multipoles $G^j_{\mu,\nu}$ vanish if $\mu$ and $\nu$ have different parity.

Below we present explicit expressions for the parameter $G^j_{\mu,\nu}$ for the most simple cases $j = 0, 1$. For $S$-state the parameter $P^{(000)}_n$ is given by eq. (A12) which leads to

$$
G^0_{0,0}(\xi, \xi') = \sum_{n=0}^{\infty} \frac{1}{(2n + 1)!} \left( \frac{\rho_1 \rho_2 Q^2}{R^2 + R'^2} \right)^n P_n (w) H^{(1)}_{2n+2} (Q \sqrt{R^2 + R'^2}),
$$

(45)

where $w = (\rho_1^2 + \rho_2^2)/(2\rho_1\rho_2)$ and $P_n (w)$ denotes the Legendre polynomial. For $P$-state ($j = 1$) there are three multipoles: $G^1_{0,0}$, $G^1_{1,1} = -(G^1_{-1,-1})^*$, $G^1_{1,-1} = (G^1_{-1,1})^*$. These coefficients correspond to the states with different spatial parity [11]. Namely, $G^1_{0,0}$ is the pseudotensor parity multipole (state $P^{even}$), and $G^1_{1,\pm 1}$ are polar tensor multipoles (state $P^{odd}$). We present here only the expression for $G^1_{0,0}$,

$$
G^1_{0,0}(\xi, \xi') = \frac{8\pi^2}{R^2 + R'^2} \left( \frac{\rho_1^2 - \rho_2^2}{\rho_1 \rho_2} \right) \sum_{n=0}^{\infty} \frac{1}{(2n + 2)!} \left( \frac{\rho_1 \rho_2 Q^2}{R^2 + R'^2} \right)^n P'_n (w) \times H^{(1)}_{2n+2} (Q \sqrt{R^2 + R'^2}),
$$

(46)

where $P'_n (w) = dP_n (w)/dw$. 

11
V. THE HYPERSPHERICAL EXPANSION OF THE MULTIPOLY COEFFICIENTS

The hyperspherical form of the multipole coefficients can be derived based on the following expansion of the three-body free Green function [8]

\[
H(1)^{2}(Q|R' - R|) = 4 \frac{(QRR')^{2}}{(QRR')^{2}} \sum_{n=0}^{\infty} (n + 2) C_{n}^{2}(\hat{R} \cdot \hat{R}') J_{n+2}(QR) H_{n+2}^{(1)}(QR'), \quad R < R', \quad (47)
\]

where \( \hat{R} \cdot \hat{R}' = p/(RR') \) and \( p \) is defined in (36); \( C_{n}^{2}(\hat{R} \cdot \hat{R}') \) is \( n \)-th order Gegenbauer polynomial [8]. If \( R > R' \) then the substitution \( R \leftrightarrow R' \) must be made in (47).

According the definition (35), the expression for the multipole coefficients can be written as

\[
G_{j}^{\mu, \nu}(\xi; \xi') = \frac{1}{(QRR')^{2}} \sum_{n=0}^{\infty} h_{n}^{(j\mu\nu)} J_{n+2}(QR) H_{n+2}^{(1)}(QR'), \quad R < R', \quad (48)
\]

where \( J_{n+2}(QR) \) is Bessel function and the functions \( h_{n}^{(j\mu\nu)} \) are defined by the integral

\[
h_{n}^{(j\mu\nu)} = 4(n + 2) \int C_{n}^{2}(\hat{R} \cdot \hat{R}') [D_{j\mu\nu}^{\dagger}(\Omega'')^{*}] d^{3}\Omega''. \quad (49)
\]

In order to calculate this integral we note that the Gegenbauer polynomial in (47) is proportional to the scalar product of six-dimensional hyperspherical harmonics [8, 12],

\[
C_{n}^{2}(\hat{R} \cdot \hat{R}') = \frac{\pi^{2}}{2(n + 2)} (\hat{Y}_{n}(\hat{R}) \cdot \hat{Y}_{n}(\hat{R}')). \quad (50)
\]

It is convenient to define harmonics \( Y_{n} \) to be the eigenfunctions of the angular momentum operators corresponding to the Jacobi vectors \( \mathbf{r}_{1} \) and \( \mathbf{r}_{2} \). In this approach, six-dimensional spherical harmonics are proportional to the product of conventional three-dimensional harmonics depending on the spherical angles of unit vectors \( \hat{\mathbf{r}}_{1} \) and \( \hat{\mathbf{r}}_{2} \),

\[
Y_{nlmm'}(\hat{\mathbf{r}}) = C_{q}^{(n-2q-l,l)}(\alpha) Y_{lm}(\hat{\mathbf{r}}_{1}) Y_{nm'}(\hat{\mathbf{r}}_{2}), \quad (51)
\]

where the functions \( C_{q}^{(n-2q-l,l)}(\alpha) \) depending on the hyperangle \( \alpha \) are defined by eq. (B2) of Appendix B.

The expression (B11) for the scalar product of six-dimensional harmonics contains the product of two Legendre polynomials depending on \( (\hat{\mathbf{r}}_{1} \cdot \hat{\mathbf{r}}_{1}') \) and \( (\hat{\mathbf{r}}_{2} \cdot \hat{\mathbf{r}}_{2}') \). Thus, in order to calculate the integral (49) it is necessary to decompose the product of two Legendre polynomials into a combination of angular functions corresponding to the states with well-defined
values of the total angular momentum $j$. This can be done by expressing the Legendre polynomials via three-dimensional spherical harmonics. Next, the product of spherical harmonics can be re-written in terms of bipolar harmonics,

$$P_l(\hat{r}_1 \cdot \hat{r}_1') P_{l'}(\hat{r}_2 \cdot \hat{r}_2') = \sum_{j=|l-l'|}^{l+l'} (-1)^{l+l'-j} \left( C_{lj}^{ll'}(\hat{r}_1, \hat{r}_2) \cdot C_{lj'}^{ll'}(\hat{r}_1', \hat{r}_2') \right),$$

(52)

where the bipolar harmonics $C_{lj}^{ll'}(\hat{r}_1, \hat{r}_2)$ are tensor product of two spherical harmonics $\hat{r}$.

$$C_{jl}^{ll'}(\hat{r}_1, \hat{r}_2) = \sum_{m,m'} C_{lm}^{j\mu} C_{l'm'}^{m\nu} C_{lm'}(\hat{r}_1) C_{l'm'}(\hat{r}_2).$$

(53)

Here, $C_{lm} = \sqrt{4\pi/(2l+1)} Y_{lm}$ are modified spherical harmonics and $C_{lm}^{j\mu}$ are Clebsch-Gordan coefficients. The scalar product of bipolar harmonics does not depend on the choice of the coordinate frame in which it is calculated. Let this frame be $BF'$, then

$$\left( C_{jl}^{l'l'}(\hat{r}_1, \hat{r}_2) \cdot C_{jl}^{l'l'}(\hat{r}_1', \hat{r}_2') \right) = \sum_{\nu} (-1)^{\nu} [C_{jl}^{l'l'}(\hat{r}_1, \hat{r}_2)][BF'] [C_{jl}^{l'l'}(\hat{r}_1', \hat{r}_2')][BF']$$

$$= \sum_{\mu,\nu} (-1)^{\nu} [C_{jl}^{l'l'}(\hat{r}_1, \hat{r}_2)][BF'] [C_{jl}^{l'l'}(\hat{r}_1', \hat{r}_2')][BF] D_{\mu,\nu}^j(\Omega''),$$

(54)

where the subscript $BF$ ($BF'$) denotes the coordinate frame in which the components must be calculated. The second identity follows from the tensor transformation rule under the rotation of the coordinate frame $\Omega''$. Now the integral can be easily calculated using the orthogonality of $D$-functions,

$$h_{n}^{(j\mu\nu)} = (-1)^{n-j+\nu} \frac{4\pi^3}{2j+1} \sum_{q,l=0} (2l+1) (2[n-2q-l]+1) C_q^{(n-2q-l,1)}(\alpha) C_q^{(n-2q-l,1)}(\alpha')$$

$$\times [C_{jl}^{(n-2q-l)}(\hat{r}_1, \hat{r}_2)][BF'] [C_{jl}^{(n-2q-l)}(\hat{r}_1, \hat{r}_2)][BF]$$

(55)

where the indices $q, l$ take non-negative integer values so that $n-2q-l \geq 0$. To derive the explicit form of $h_{n}^{(j\mu\nu)}$ it is necessary to specify the gauge convention. The only exception is the case of $j = 0$ (S-wave part of the expansion), when the coefficient $h_{n}^{(000)}$ is scalar

$$h_{2n}^{(000)} = 4\pi^3 \sum_{l=0}^{n} (2l+1) C_{n-l}^{(l,1)}(\alpha) C_{n-l}^{(l,1)}(\alpha') P_l(\cos \theta) P_l(\cos \theta').$$

(56)

Note that the coefficients $h_{n}^{(000)}$ with odd $n$ vanish, $h_{2n+1}^{(000)} = 0$. 

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For $j > 0$ we use the angle-bisector gauge (see fig. 2 above). In that gauge, the components of bipolar harmonics in (55) have the form

$$
[C_{j
u}^{l,(n-2q-l)}(\hat{r}_1, \hat{r}_2)]_{BF} = C_{j\mu}^{l,(n-2q-l)}(\pi/2, -\theta/2, \pi/2, \theta/2)
$$

$$
= \sum_m C_{lm,(n-2q-l),(\mu-m)}^j C_{lm}(\pi/2, -\theta/2) C_{(n-2q-l),(\mu-m)}(\pi/2, \theta/2). \quad (57)
$$

Note that the explicit expression for the spherical harmonics $C_{lm}(\pi/2, \theta)$ is rather simple [9]

$$
C_{lm}(\frac{\pi}{2}, -\frac{\theta}{2}) = \begin{cases} 
(-1)^{(l+m)/2} e^{-i\frac{m\theta}{2}} \sqrt{(l+m-1)!!(l-m-1)!!}, & l + m = \text{even} \\
0, & l + m = \text{odd}. 
\end{cases} \quad (58)
$$

From this identity and the symmetry properties of Clebsch-Gordan coefficients it follows that $h_{n}^{(j\mu\nu)}$ are non-zero only for $n, \mu$ and $\nu$ having the same parity.

For $j = 1$ and $\mu = \nu = 0$ it is convenient to use the reduction formula for bipolar harmonics [13],

$$
[C_{10}^{l}(\hat{r}_1, \hat{r}_2)]_{BF} = \frac{i(-1)^{l+1} \sqrt{3}}{\sqrt{l(l+1)(2l+1)}} P_1^l(\theta), 
$$

where $P_1^l(\theta)$ is the associated Legendre polynomial, $P_1^l(\theta) = -\sin \theta P'_1(\cos \theta)$. As a result, the coefficient (55) assumes the form

$$
h_{2n}^{(100)} = 4\pi^3 \sum_{l=1}^{n} \frac{2l+1}{l(l+1)} C_{n-l}^{(l,l)} C_{n-l}^{(l,l)} P_1^l(\theta) P_1^l(\theta'), \quad (60)
$$

Coefficients with odd index $n$ vanish, $h_{2n+1}^{(100)} = 0$.

VI. CONCLUSION

In the presented paper the perturbation theory was applied to the calculation of the wave function of the three-body system in which the potential $U$ of the inter-particle interaction is small comparing to the kinetic energy.

The expression for the wave function in the zeroth- and first-order approximation with respect to $U$ is given by eq (19). The problem of the calculation of the matrix elements between the continuum state wave function and the wave function having well-defined angular momentum quantum numbers has been considered in Sec. III. The calculation procedure leads to the appearance of twelve-dimensional integrals (see eq. (23)) which, in the most important particular case of an isolated system, can be reduced to six-dimensional integrals,
see eq. (31). The reduction was achieved by employing the technique of collective multipole
expansions in terms of Wigner $D$-functions (see eqs. (24) and (26)) describing the rotation
from the body-fixed frame (BF) to the laboratory-fixed frame (LF).

The collective multipole coefficients (CMC) of the expansion of the Green function of
the system of three free particles were calculated in Sec. IV and V. The two different ap-
proaches were used for the calculation of CMC. The first one (Sec. IV) is the straightforward
computation of the integral defining CMC using BF and LF corresponding to the so-called
angle-bisector gauge (see fig. 2). The expression for CMC in that approach is given by
eq. (43).

The second (hyperspherical) approach was based on the expansion of the three-body free
Green function over the basis set of six-dimensional hyperspherical harmonics. Note that
those were not conventional harmonics as defined in [8, 12] but the set of harmonics labeled
by the individual angular momenta quantum numbers of particles [14]. The expression for
CMC was then extracted from the series by using some specific gauge convention (eqs. (48),
(55) of Sec. V).

The advantage of the straightforward approach is that the resulting series representation
of CMC is simpler compared to that of the hyperspherical approach. Also, it remains
valid in the whole shape space while the hyperspherical series diverge at the configuration
when $R = R'$. Nevertheless, the hyperspherical representation can be more favorable if the
potential energy can be factorized in terms of hyperspherical coordinates. In this case the
many-dimensional integrals of the perturbation theory reduce to the one-dimensional form.

Both representations of CMC are series of Hankel functions $H^{(1,2)}_n$ depending on hyperra-
dial variables multiplied with weight functions depending on the hyperangles. These series
converge rather well. For example, at $Q = 10$, $R = 1$, $R = 2$, $\alpha = \alpha' = \theta = \theta' = 45^o$ the
number of terms in series which are needed to achieve the accuracy of $10^{-6}$ is about thirty.
The convergence rate decreases as $Q$ and/or $R$’s increase. The same behavior is observed as
the configuration triangles (see fig. 1) become narrower at the same $Q$ and $R$’s.

In general case of $j > 0$, CMC are functions of six variables, i.e. two times the dimen-
sionality of the shape space of three particles. Surprisingly, from eq. (45) it follows that
CMC corresponding to an $S$-state (with $j = 0$) depends only on three variables. (Note that
this property of $S$-state CMC is not seen from (56) of the hyperspherical approach.) Such
property of $S$-state CMC was already noticed in [7] where the collective multipole expansion
of the product of three-dimensional plane waves has been considered. This fact still needs 
some physical explanation.

Currently, the work on the application of the developed theory to the problem of the 
three-particle fragmentation process is in progress.

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APPENDIX A: THE INTEGRATION OF $p^n$ OVER EULER ANGLES

In order to calculate the integral (44) we employ the expression for Wigner D-functions 
in terms of Euler angles, $D_{\mu,\nu}^j(\Omega) = e^{-i(\alpha+\gamma)} d_{\mu,\nu}^j(\beta)$. First, we calculate the integral over the 
angles $\alpha$ and $\gamma$,

$$I_{\mu\nu} = \int_0^{2\pi} \int_0^{2\pi} e^{i(\mu \alpha + \nu \gamma)} (a_1 \sin(\alpha + \gamma + \delta_1) - a_2 \sin(\alpha - \gamma + \delta_2))^n d\alpha d\gamma, \quad (A1)$$

This integral can be calculated using the exponential representation of sine functions. It 
turns out that the integral is non-zero only for indices $n, \mu, \nu$ having the same parity. 
Omitting details of routine transformations, we write

$$I_{\mu\nu} = 4\pi^2 (-1)^{\frac{n+\mu}{2}} e^{-i\delta_1} e^{-i\delta_2} \frac{n!}{(2i)^n} \sum_k \frac{\alpha_1^{n+\mu-2k} \alpha_2^{2k+\nu}}{k! (k + \nu)! (\frac{n-\mu}{2} - k)! (\frac{n+\nu}{2} - k)!}, \quad (A2)$$

where the sum runs over all non-negative values of $k$ at which factorials remain finite. Note 
that factorials and indices $\bar{\mu}, \bar{\nu}$ in eq. (A2) are always integer numbers (as was mentioned 
above),

$$\bar{\mu} = \frac{\mu + \nu}{2}, \quad \bar{\nu} = \frac{\mu - \nu}{2}. \quad (A3)$$

Using the explicit form of the function $d_{\mu,\nu}^j(\beta)$ we can integrate (A2) over $\beta$ term by term. 
The partial integrals are

$$\int_0^\pi \alpha_1^{n-\nu-2k} \alpha_2^{2k+\nu} d_{\mu,\nu}^j(\beta) \sin \beta d\beta = 2\sqrt{(j + \mu)! (j - \mu)! (j + \nu)! (j - \nu)!}$$

$$\times \sum_q \beta_1^{n-\nu-2k} \beta_2^{2k+\nu} (-1)^{j-\nu+q} (q + n + \nu - 2k)! (j - q - \nu + 2k)!$$

$$\times q! (j - \mu - q)! (j - \nu - q)! (\nu + \mu + q)! (j + n + 1)!. \quad (A4)$$

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Substituting eq. (A4) into eq. (A2) we can re-write the summation over \( k \) in (A2) as

\[
\sum_k \left( \frac{\rho_2}{\rho_1} \right)^{2k} \frac{(q+n+\nu-2k)! (j-q-\nu+2k)!}{k! (k+\nu)! (\frac{n+\nu}{2} - k)! (\frac{n+\nu}{2} - k)!} = \sum_k \left( \frac{\rho_2}{\rho_1} \right)^{2k} \times \frac{(2k+\mu-\nu-1)! (n-\mu-2k-1)! (q+n+\nu-2k)! (j-q-\nu+2k)!}{k! (k+\nu)! (\frac{n+\nu}{2} - k)! (\frac{n+\nu}{2} - k)! (n-\mu-2k)! (\mu-\nu+2k)!}.
\]

(A5)

The last multiplicand on rhs on this equation can be presented in a compact differential form

\[
\frac{(q+n+\nu-2k)! (j-q-\nu+2k)!}{(n-\mu-2k)! (\mu-\nu+2k)!} = (-1)^{q+\mu+\nu} \partial^{j-\mu-q} t^{n+j+1} \partial^{\nu+q} t^{-n+\mu+2k-1}]_{t=1}.
\]

(A6)

Substituting this identity into (A5) we put derivatives outside the summation. Thereby, it evaluates in closed form

\[
\sum_k (\ldots) = (-1)^{\mu+\nu+q} 2^{\frac{n-\nu}{2}} \frac{(\mu-\nu-1)! (n-\mu-1)!}{(\frac{n+\nu}{2})!} \times \partial^{j-\mu-q} t^{n+j+1} \partial^{\mu+\nu} = t^{n+j+1-m}
\]

\[
\times \sum_m m! (n+j+1)! \partial^{j+\nu-m} \sum_q q! (j-\nu+q)! (j-\mu-q)! (\nu+q)! (\mu-q)! (n+j+1-m)!
\]

(A7)

The final step is to rearrange the exterior summation over \( q \),

\[
\sum_q \frac{1}{q! (j-\mu-q)! (j-\nu-q)! (\nu+\mu+q)!} \partial^{j-\mu-q} t^{n+j+1} \partial^{\mu+\nu} = t^{n+j+1-m}
\]

\[
\times \sum_m m! (n+j+1)! \partial^{j+\nu-m} \sum_q q! (j-\nu+q)! (\nu+\mu+q)! (j-\mu-q-m)!
\]

(A8)

Here, the decouple sum over \( q \) evaluates to a closed form,

\[
\sum_q (\ldots) = \frac{(2j-m)!}{(j+\mu)! (j-\nu)! (n-\mu-m)! (j+\nu-m)!}.
\]

(A9)

Collecting above eqs. (A2), (A4), (A7) – (A9) we finally write the expression for the integral (44),

\[
P_n^{(j,\mu)} = 8\pi^2 i^n (-1)^{j+\frac{\mu+\nu}{2}} \rho_1^2 e^{-i\delta_1 (\mu+\nu)/2} \left( \frac{\rho_2}{\rho_1} \right)^{\frac{(\mu-\nu)/2}{2}} \frac{(\mu-\nu-1)! (n-\mu-1)!}{(n+\nu)!} \times \sqrt{\frac{(j-\mu)! (j+\nu)!}{(j+\mu)! (j-\nu)!}} \sum_m m! (j-\mu-m)! (j+\nu-m)! (n+j+1-m)!
\]

\[
\times \partial^{j+\nu-m} \mu^{-n-1} 2F_1 \left( \frac{1+\mu-\nu}{2}, -\frac{n+\nu}{2}; \frac{1+\mu-n}{2}; \frac{(t\rho_2)^2}{\rho_1^2} \right) \bigg|_{t=1}.
\]

(A10)
Note that the derivative can be written as a combination of Gauss hypergeometric functions,

\[ \partial^j + \nu - m \mu - n - 1 \left( \frac{1}{2}, -\frac{n + \nu}{2}, \frac{1 + \mu - n}{2}; \frac{(\rho_2)^2}{\rho_1^2} \right) \bigg|_{t=1} \]

\[ = \sum_{\alpha=(j+\nu-m), (j+\nu-m)-1,...} \frac{(-1)^\alpha 2^{2\alpha-j-\nu+m}(j+\nu-m)!}{(2\alpha-j-\nu+m)!(j+\nu-m-\alpha)!} \times \left( \frac{1-\mu+n}{2} \right)_\alpha \left( \frac{1}{2}, -\frac{n+\nu}{2}, \frac{1+\mu-n}{2} - \alpha; \frac{\rho_2^2}{\rho_1^2} \right), \quad (A11) \]

where \( (\frac{1-\mu+n}{2})_\alpha \) denotes Pochhammer symbol [15].

Using eq. (A10), one can easily calculate the coefficient \( P_{2n}(000) \) corresponding to an \( S \)-state,

\[ P_{2n}(000) = 8\pi^2 \rho_1^{2n} (\rho_1 \rho_2) (2n-1)!! (2n+1)!! \left( \frac{1}{2}, -n, \frac{1}{2} - n; \frac{\rho_2^2}{\rho_1^2} \right). \quad (A12) \]

Here, the hypergeometric function reduces to the Legendre polynomial which leads to eq. (45). For \( P^e \)-state with pseudotensor parity the non-zero parameter is

\[ P_{2n+1}^{(100)} = -16\pi^2 \left( \rho_1 \rho_2 \right)^n (\rho_1 \rho_2) (2n+2)!! (n+1) t^{-n-1} P_n \left( \frac{\rho_1^2 + t^2 \rho_2^2}{2t \rho_1 \rho_2} \right) \bigg|_{t=1}. \quad (A13) \]

Calculating the derivative in this identity we arrive at eq. (46) of the main text. Note that both above parameters with odd index vanish, i.e. \( P_{2n+1}^{(000)} = P_{2n+1}^{(100)} = 0. \)

**APPENDIX B: THE SIX-DIMENSIONAL HYPERSPHERICAL HARMONICS AND THEIR PROPERTIES**

For the sake of completeness below we summarize the most important properties of the set of six-dimensional hyperspherical harmonics which are eigenfunctions of the particle’s angular momentum operators. The derivation of the results can be found, e.g. in [14].

The scalar product of two hyperspherical harmonics is defined by

\[ (Y_n(\hat{R}) \cdot Y_n(\hat{R}')) = \sum_{l=0}^{n} \sum_{q=0}^{q_{\text{max}}} \sum_{mm'} Y^*_{nqlnmm'}(\hat{R}) Y_{nqlm'm'}(\hat{R}') = \sum_{ql} \left( \frac{2l+1}{4\pi} \right) \]

\[ \times (2[n-2q-l]+1) C_q^{(n-2q-l,1)}(\alpha) C_q^{(n-2q-l,1)}(\alpha') P_l(\hat{r}_1 \cdot \hat{r}_1') P_{N-2q-l}(\hat{r}_2 \cdot \hat{r}_2'), \quad (B1) \]

where \( q_{\text{max}} \) is the integer part of the ratio \( (n-l)/2 \) and the hyperangle \( \alpha \) is defined in [34].
The functions $C_{q}^{(n-2q-l,l)}$ are defined as

$$C_{q}^{(l',l)}(\alpha) = \sqrt{\frac{2l'+3}{\pi (2q+2l'+1)!}} \frac{(2q+l+l'+2)! q! (q+l+l'+1)!}{(2q+2l+1)!! (2q+2l'+1)!!} \times 2^q (\sin \alpha)^{l'} (\cos \alpha)^l P_{q}^{(l'+1/2,l+1/2)}(\cos 2\alpha), \quad (B2)$$

where $P_{q}^{(a,b)}$ is Jacobi polynomial. Above functions are orthonormal,

$$\int_{0}^{\pi/2} C_{q}^{(l',l)}(\alpha) C_{q'}^{(l',l)}(\alpha) \frac{\sin^2 2\alpha}{4} d\alpha = \delta_{q,q'}, \quad (B3)$$

The hyperspherical harmonics defined by eq. (51) are orthonormal,

$$\int Y_{nqlmm'}^{*} (\hat{R}) Y_{nqlmm'} (\hat{R}) d\tilde{\Omega} = d_{n,n} d_{q,q} d_{l,l} d_{m,m} d_{m',m'}, \quad (B4)$$

where $d\tilde{\Omega}$ is the surface elements of the six-dimensional hypersphere, which can be written as

$$d\tilde{\Omega} = \frac{\sin^2 2\alpha}{4} \sin \theta_1 \sin \theta_2 d\alpha d\theta_1 d\theta_2 d\phi_1 d\phi_2, \quad (B5)$$

where $\theta_1, \phi_1$ are three-dimensional spherical angles of the unit vectors $\hat{r}_1$. Note that the total solid angle in the six-dimensional space is

$$\int_{S_6} d\tilde{\Omega} = \pi^3, \quad (B6)$$

where $S_6$ is the six-dimensional hypersphere of the unit radius.

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