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2004 J. Phys. A: Math. Gen. 37 701

(http://iopscience.iop.org/0305-4470/37/3/013)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 701–718 PII: S0305-4470(04)62818-6

Boundary conditions on wavefunctions for three bodies at singular configurations

Toshihiro Iwai and Toru Hirose

Department of Applied Mathematics and Physics, Kyoto University, Japan

Received 28 April 2003, in final form 30 September 2003
Published 7 January 2004
Online at stacks.iop.org/JPhysA/37/701 (DOI: 10.1088/0305-4470/37/3/013)

Abstract

Singular configurations have long been out of consideration in the study of many-particle systems. In this paper we show that a group theoretical method can provide boundary conditions on wavefunctions at singular configurations of many particles. The consequences of this method are qualitatively stated as follows. (i) If the projection of angular momentum on an axis does not vanish, the particles will not be aligned on the axis, i.e. the wavefunction vanishes at collinear configurations along the axis. (ii) If the total angular momentum does not vanish, the simultaneous collision at a point will not take place, i.e. the wavefunction vanishes at the configuration of simultaneous collision. Furthermore, on the assumption of analyticity of the wavefunction at singular configurations, the behaviour of the wavefunction around the singular configurations shows that (a) the larger the projection of angular momentum on an axis becomes, the less the particles are likely to be aligned on the line, and that (b) the more the total angular momentum grows, the less likely the particles are to collide at a point. The proof is carried out for three-body systems by transforming the power series expansion of a wavefunction into a Fourier series expansion in terms of the angular momentum eigenfunctions, in both cases of collinear configurations and of the triple collision, without reference to the Hamiltonian operator. These results are described quantitatively in terms of the angular momentum quantum numbers in propositions 1 and 3 in the text.

PACS numbers: 02.40.−k, 02.20.−a, 31.15.−p

1. Introduction

The centre-of-mass system of many particles admits a natural action of the rotation group $SO(3)$. The phrase 'singular configurations', as used in the title of this paper, means those configurations at which the rotation group $SO(3)$ has non-trivial isotropy subgroups. Practically, the singular configurations under consideration are collinear configurations and a multiple collision. If singular configurations are removed from the centre-of-mass system, the restricted centre-of-mass system is made into an $SO(3)$ bundle [1], and the bundle picture works well in the study of quantum mechanics of many bodies [2–7]. For example, reducing the rotational degrees of freedom is well performed in this picture. In fact, we can form complex vector bundles associated with the $SO(3)$ bundle, on which reduced quantum systems are to be defined. However, if we want to take singular configurations into account, the bundle picture fails to work.

One of the authors (TI) has presented a method [8] for treating wavefunctions at singular configurations. We call this method the Peter–Weyl method. This nomenclature comes from the Peter–Weyl theorem on the unitary irreducible representations of compact Lie groups. This theorem turns out to provide a method for expanding wavefunctions into Fourier series with respect to the symmetry described by the compact Lie group. Since the Peter–Weyl method works irrespective of whether the Lie group acts freely on a manifold in question (i.e. isotropy subgroups are trivial everywhere) or not, we can apply the method to study the behaviour of wavefunctions at singular configurations.

Since the kinetic operator has singularity at singular configurations [4], the boundary behaviour of wavefunctions at singular configurations is needed for this study. Mitchell and Littlejohn [9] studied the boundary behaviour of wavefunctions for three bodies at collinear configurations by means of the $SO(2)$ representations, but did not consider the boundary behaviour at a multiple collision. In this paper, three-body systems are also treated to obtain explicitly boundary conditions on wavefunctions both at collinear configurations and at a triple collision, by means of the group representation theory.

The organization of this paper is as follows. Section 2 is concerned with the centre-of-mass system. In section 3 we give a brief review of the Peter–Weyl method, according to which we can discuss Fourier series expansions of wavefunctions and the decomposition of the Hilbert space of wavefunctions. In section 4, the Peter–Weyl method is applied to three-body systems. In practice, Fourier analysis is performed for wavefunctions with respect to D functions associated with the total angular momentum operator. Section 5 is concerned with boundary conditions on wavefunctions at collinear configurations. It is shown that if the projection of angular momentum on an axis does not vanish, the particles will not be aligned on the axis, i.e. the wavefunction vanishes at collinear configurations along the axis. Furthermore, on the assumption that the wavefunction is analytic in a neighbourhood of the collinear configuration, it will be shown that the larger the angular momentum around an axis becomes, the less the particles are likely to be aligned on the axis (see proposition 1). To show this fact, the power series expansion of a wavefunction is brought into the form of a Fourier series expansion. Section 6 deals with boundary conditions on wavefunctions at the triple collision. It will be shown, as expected, that if the total angular momentum does not vanish, the simultaneous collision at a point will not take place, i.e. the wavefunction vanishes at the configuration of triple collision. Furthermore, it turns out that if a wavefunction is analytic in the neighbourhood of the triple collision, then the more the total angular momentum grows, the less the particles are likely to collide at a point (see proposition 3). For the proof of this fact, the Clebsch–Gordan formula is used intensively. It is to be noted that the boundary behaviour of wavefunctions observed in sections 5 and 6 is independent of the Hamiltonian as long as the Hamiltonian admits wavefunctions satisfying the assumption of the propositions. In fact, the observation is made by means of transformation group theory only. Section 7 includes remarks on the realization of the Clebsch–Gordan formula in terms of solid harmonics.

2. The centre-of-mass system

Let $\boldsymbol{x}_i$ and m_i, with $i = 1, \ldots, N$, be position vectors and masses of point particles in $\mathbf{R}^3$, respectively. Then the configurations of the point particles are denoted by $x = (\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$, which may be viewed as $3 \times N$ matrices. The centre-of-mass system M is defined to be

$$M = \left\{ x = (\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) | \boldsymbol{x}_i \in \mathbf{R}^3, \sum_{i=1}^{N} m_i \boldsymbol{x}_i = 0 \right\}. \tag{1}$$

The configurations of particles are characterized by the linear subspaces

$$F_x := \operatorname{span}\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}. \tag{2}$$

According to whether $\dim F_x = 0, 1, 2, 3$, the configuration x of the particles is point-like, collinear, planar or spatial. Thus M is broken up into four:

$$M = \bigcup_{k=0}^{3} M_k \qquad M_k := \{x \in M | \dim F_x = k\} \quad k = 0, 1, 2, 3. \tag{3}$$

The centre-of-mass system admits an $SO(3)$ action:

$$\Phi_g(x) = gx = (g\boldsymbol{x}_1, g\boldsymbol{x}_2, \ldots, g\boldsymbol{x}_N) \qquad g \in SO(3), x \in M. \tag{4}$$

The isotropy subgroup G_x of $G = SO(3)$ at $x \in M$ is defined, as usual, to be $G_x = \{g \in G | gx = x\}$. We can show easily that $SO(3)$ acts on $M_2 \cup M_3$ freely, that is, if $\Phi_g(x) = x$ for $x \in M_2 \cup M_3$, then $g = I$ (the 3×3 identity matrix), which means that the isotropy subgroups are trivial, $G_x = \{I\}$, on $M_2 \cup M_3$. However, on M_1 and on M_0, the isotropy subgroups are non-trivial; at $x \in M_1$ and at $x \in M_0$, they are isomorphic with $SO(2)$ and with $SO(3)$, respectively. Configurations in $M_0 \cup M_1$ are called singular, which are point-like or collinear. Depending on the dimensionality of the isotropy subgroups G_x, orbits $\mathcal{O}_x$ of G through $x \in M$ are classified into three; according to whether $G_x \cong \{I\}, SO(2)$, or $SO(3)$, the dimension of $\mathcal{O}_x$ is 3, 2 or 0.

On restricting M to $\dot{M} := M_2 \cup M_3$, we can make $\dot{M}$ into a principal fibre bundle $\dot{M} \to \dot{Q} := \dot{M}/SO(3)$ [1], since $SO(3)$ is compact and since $SO(3)$ acts on $\dot{M}$ freely. However, the total space M cannot be made into a fibre bundle, since the orbit space $Q := M/SO(3)$ is not a manifold. To see what occurs in this case, we take a three-body system, for example. As is well known, the Jacobi vectors in this case are defined to be

$$\boldsymbol{r}_1 := \sqrt{\frac{m_1 m_2}{m_1 + m_2}} (\boldsymbol{x}_2 - \boldsymbol{x}_1) \qquad \boldsymbol{r}_2 := \sqrt{\frac{m_3(m_1 + m_2)}{m_1 + m_2 + m_3}} \left(\boldsymbol{x}_3 - \frac{m_1 \boldsymbol{x}_1 + m_2 \boldsymbol{x}_2}{m_1 + m_2} \right). \tag{5}$$

Thus, M is viewed as the linear space formed by all the pairs $(\boldsymbol{r}_1, \boldsymbol{r}_2)$, or as the space of 3×2 matrices. Then we can regard $\dot{M} = M_2 (M_3 = \emptyset)$ as the space of 3×2 matrices of maximal rank. M_1, M_0 are the space of 3×2 matrices of rank one and of rank 0, respectively. Singular configurations sitting in M_1 and M_0 form the boundary of the regular configurations in M_2. Note that $\dim \dot{M} = 6$, $\dim M_1 = 4$, and $\dim M_0 = 0$ for three-body systems.

In terms of the Jacobi vectors $\boldsymbol{r}_1, \boldsymbol{r}_2$, we can realize the projection $\pi : M \to Q$ as follows

$$(\boldsymbol{r}_1, \boldsymbol{r}_2) \mapsto (w_1, w_2, w_3) := (\|\boldsymbol{r}_1\|^2 - \|\boldsymbol{r}_2\|^2, 2\boldsymbol{r}_1 \cdot \boldsymbol{r}_2, 2\|\boldsymbol{r}_1 \times \boldsymbol{r}_2\|) \tag{6}$$

which shows that the orbit space Q is homeomorphic with the closed half space of $\mathbf{R}^3$:

$$Q \cong \mathbf{R}^3_{\geqslant 0} := \{(w_1, w_2, w_3) \in \mathbf{R}^3 | w_3 \geqslant 0\}. \tag{7}$$

The subspace $\dot{M}$, which is open and dense in M, maps to the open half space $\dot{Q} \cong \mathbf{R}^3_{>0} := \{(w_1, w_2, w_3) \in \mathbf{R}^3 | w_3 > 0\}$, and the subspace $M_1 \cup M_0$ to the plane determined by $w_3 = 0$, which forms the boundary of the orbit space $Q \cong \mathbf{R}^3_{\geqslant 0}$.

For four or more bodies, the orbit space $M/SO(3)$ is difficult to study. Littlejohn and co-workers have studied those spaces for four and five bodies by means of 'kinetic rotations' [10, 11].

In general, wavefunctions of a three-body system are described in terms of six independent variables, three of which are the Euler angles and the remaining three are internal coordinates (or shape parameters). We note here that $\dim \dot{M} = 6$ and $\dim M_1 = 4$. A question then arises as to how the wavefunction for three bodies behaves when the configuration $x \in \dot{M}$ is approaching a collinear one (i.e. $x \to x_0 \in M_1$). We may expect that the wavefunction should be subject to some kind of boundary conditions at the collinear configuration. Although there are few occasions when singular configurations take place, they are allowed to occur, so that we have to consider what happens in wavefunctions in the neighbourhood of singular configurations.

3. Fourier analysis of wavefunctions

This section is a review of the Peter–Weyl method [8], which will provide the Fourier analysis of wavefunctions. Let M be a manifold on which a compact Lie group G acts. Let μ_M be a G-invariant measure on M. The space $L^2(M)$ of square integrable functions on M is the Hilbert space we take as the space of wavefunctions, in which the G is represented unitarily through $(U(g)f)(x) = f(g^{-1}x)$, $g \in G$, $x \in M$. The representation $g \mapsto U(g)$ is then decomposed into unitary irreducible representations. To describe the decomposition, we make a brief review of the Peter–Weyl theorem.

Let μ_G and $L^2(G)$ denote the normalized invariant measure on G and the space of square integrable functions on G with respect to μ_G, respectively. Let $(\mathcal{H}^\chi, \rho^\chi)$ be unitary irreducible representations of G, where χ ranges over all the inequivalent representations. We denote by ρ^χ_{ij} the matrix elements of the representation ρ^χ with respect to an orthonormal basis e^λ_i of $\mathcal{H}^\chi$, where $i, j = 1, \ldots, d_\chi$, with $d_\chi = \dim \mathcal{H}^\chi$. The Peter–Weyl theorem states that the set of all the matrix elements $\left\{\sqrt{d_\chi}\rho^\chi_{ij}\right\}_{\chi,i,j}$ forms a complete orthonormal system in $L^2(G)$. Then any function φ of $L^2(G)$ is expanded into a Fourier series:

$$\varphi(h) = \sum_{\chi,i,j} d_\chi \rho^\chi_{ij}(h) \int_G \overline{\rho^\chi_{ij}(g)} \varphi(g) \, \mathrm{d}\mu_G(g). \tag{8}$$

We turn to wavefunctions. For a function $f \in L^2(M)$, we may view $f(hx)$ as a function on G with x fixed arbitrarily, $f_x(h) := f(hx)$, and apply the above expansion formula to f_x to obtain

$$f(hx) = \sum_{\chi,i,j} d_\chi \rho^\chi_{ij}(h) \int_G \overline{\rho^\chi_{ij}(g)} f(gx) \, \mathrm{d}\mu_G(g) \tag{9}$$

$$= \sum_{\chi,i} d_\chi \int_G \rho^\chi_{ii}(g) f(g^{-1}hx) \, \mathrm{d}\mu_G(g). \tag{10}$$

In particular, for $h = e$, we have

$$f(x) = \sum_{\chi,i} d_\chi \int_G \rho^\chi_{ii}(g) f(g^{-1}x) \, \mathrm{d}\mu_G(g). \tag{11}$$

This suggests that we define the operators P_i^χ on $L^2(M)$ by

$$P_i^\chi := d_\chi \int_G \rho_{ii}^\chi(g) U(g) \, \mathrm{d}\mu_G(g). \tag{12}$$

Furthermore, a straightforward calculation shows that

$$\left(P_i^\chi\right)^\dagger = P_i^\chi \qquad P_i^\chi P_j^{\chi'} = \delta^{\chi\chi'} \delta_{ij} P_i^\chi \tag{13}$$

which means that P_i^χ are orthogonal projection operators. Then equation (11) provides the orthogonal direct sum decomposition

$$L^2(M) = \bigoplus_{\chi,i} \mathrm{Im}\, P_i^\chi. \tag{14}$$

Furthermore, we define the operators

$$P_{ij}^\chi := d_\chi \int_G \rho_{ij}^\chi(g) U(g) \, \mathrm{d}\mu_G(g) \tag{15}$$

which prove to satisfy that

$$\left(P_{ij}^\chi\right)^\dagger = P_{ji}^\chi \qquad P_{ij}^\chi P_{k\ell}^{\chi'} = \delta^{\chi\chi'} \delta_{jk} P_{i\ell}^\chi. \tag{16}$$

In particular, we have $P_{ii}^\chi = P_i^\chi$. Moreover, we verify that

$$\left(P_{ij}^\chi\right)^\dagger P_{ij}^\chi = P_j^\chi \qquad P_{ij}^\chi \left(P_{ij}^\chi\right)^\dagger = P_i^\chi. \tag{17}$$

It then follows that when restricted to $\mathrm{Im}\, P_j^\chi$, P_{ij}^χ provides the unitary isomorphism

$$P_{ij}^\chi : \mathrm{Im}\, P_j^\chi \xrightarrow{\sim} \mathrm{Im}\, P_i^\chi. \tag{18}$$

Furthermore, we can show that P_{ij}^χ and $U(g)$ are put together to give

$$P_{ij}^\chi U(g) = \sum_k \rho_{kj}^\chi(g^{-1}) P_{ik}^\chi \qquad U(g) P_{ij}^\chi = \sum_k \rho_{ik}^\chi(g^{-1}) P_{kj}^\chi. \tag{19}$$

The second equation of (19) implies that the map $E_j^\chi : L^2(M) \to \mathcal{H}^\chi \otimes L^2(M)$ defined by

$$E_j^\chi := \frac{1}{\sqrt{d_\chi}} \sum_{i=1}^{d_\chi} e_i^\chi \otimes P_{ij}^\chi \tag{20}$$

satisfies

$$U(g^{-1}) E_j^\chi = \rho^\chi(g) E_j^\chi. \tag{21}$$

This equation states that $\mathcal{H}^\chi$-valued functions $E_j^\chi f$ with $f \in L^2(M)$ are ρ^χ-equivariant functions;

$$\left(E_j^\chi f\right)(gx) = \rho^\chi(g) \left(E_j^\chi f\right)(x). \tag{22}$$

We here introduce the space, $L^2(M; \mathcal{H}^\chi)^G$, of square integrable equivariant $\mathcal{H}^\chi$-valued functions by

$$L^2(M; \mathcal{H}^\chi)^G := \left\{ \psi : M \to \mathcal{H}^\chi \,|\, \int_M \|\psi(x)\|^2 \, \mathrm{d}\mu_M(x) < \infty, \right.$$
$$\left. \psi(gx) = \rho^\chi(g)\psi(g),\ g \in G,\ x \in M \right\} \tag{23}$$

where $\|\cdot\|$ denotes the norm in $\mathcal{H}^\chi$. Since $\mathcal{H}^\chi \otimes L^2(M)$ is the space of $\mathcal{H}^\chi$-valued square integrable functions, we can view the operator E_j^χ as a map $L^2(M) \to L^2(M;\mathcal{H}^\chi)^G$. The adjoint operator $\left(E_j^\chi\right)^\dagger : L^2(M;\mathcal{H}^\chi)^G \to L^2(M)$ is defined, of course, through

$$\left\langle \psi, E_j^\chi f \right\rangle_{L^2(M;\mathcal{H}^\chi)^G} = \left\langle \left(E_j^\chi\right)^\dagger \psi, f \right\rangle_{L^2(M)} \qquad \psi \in L^2(M;\mathcal{H}^\chi)^G \qquad f \in L^2(M) \tag{24}$$

where the subscripts $L^2(M;\mathcal{H}^\chi)^G$ and $L^2(M)$ indicate the spaces on which the respective inner products are defined. Then we can observe that

$$\left(E_j^\chi\right)^\dagger E_j^\chi = P_j^\chi \qquad E_j^\chi \left(E_j^\chi\right)^\dagger = \mathrm{id}_{L^2(M;\mathcal{H}^\chi)^G} \tag{25}$$

where $\mathrm{id}_{L^2(M;\mathcal{H}^\chi)^G}$ denotes the identity map of $L^2(M;\mathcal{H}^\chi)^G$. The above relations imply that when restricted to $\mathrm{Im}\, P_j^\chi$, E_j^χ provides a unitary isomorphism

$$E_j^\chi : \mathrm{Im}\, P_j^\chi \xrightarrow{\sim} L^2(M;\mathcal{H}^\chi)^G \qquad j = 1, \ldots, d_\chi. \tag{26}$$

From equation (14) along with $\bigoplus_j \mathrm{Im}\, P_j^\chi \cong (\mathcal{H}^\chi)^* \otimes L^2(M;\mathcal{H}^\chi)^G$, we obtain, in conclusion,

$$L^2(M) \cong \bigoplus_\chi ((\mathcal{H}^\chi)^* \otimes L^2(M;\mathcal{H}^\chi)^G). \tag{27}$$

4. Three-body systems

In this section, we apply the Peter–Weyl method to a three-body system. The manifold M we take is the centre-of-mass system for three bodies, which is identified with the pairs of Jacobi vectors $M = \{(\boldsymbol{r}_1, \boldsymbol{r}_2)\} \cong \mathbf{R}^3 \times \mathbf{R}^3$. The rotation group $SO(3)$ acts on M in the manner $(\boldsymbol{r}_1, \boldsymbol{r}_2) \mapsto (g\boldsymbol{r}_1, g\boldsymbol{r}_2)$ with $g \in SO(3)$. We introduce the Euler angles (ϕ, θ, ψ) through

$$g = \mathrm{e}^{\phi \hat{e}_3} \mathrm{e}^{\theta \hat{e}_2} \mathrm{e}^{\psi \hat{e}_3} \qquad g \in SO(3) \tag{28}$$

where $\boldsymbol{e}_k$, $k = 1, 2, 3$, are the standard basis of $\mathbf{R}^3$ and $\hat{\boldsymbol{e}}_k$ denote the 3×3 matrices defined through $\hat{\boldsymbol{e}}_k \boldsymbol{a} = \boldsymbol{e}_k \times \boldsymbol{a}$ for $\boldsymbol{a} \in \mathbf{R}^3$. Let $D_{nm}^\ell(g)$ denote the matrix elements of unitary irreducible representations of $SO(3)$ with $\ell = 0, 1, 2, \ldots,$ and $|m|, |n| \leqslant \ell$ [12]. They are expressed as

$$D_{nm}^\ell(g) = \mathrm{e}^{-\mathrm{i}n\phi} d_{nm}^\ell(\theta)\, \mathrm{e}^{-\mathrm{i}m\psi} \tag{29}$$

where $d_{nm}^\ell(\theta)$ are given by

$$\begin{aligned} d_{nm}^\ell(\theta) &= (-1)^{n-m} \sqrt{(\ell+n)(\ell-n)(\ell+m)(\ell-m)} \\ &\quad \times \sum_{k=0}^{\ell-m} \frac{(-1)^k}{k!(\ell-n-k)!(\ell+m-k)!(n-m+k)!} \\ &\quad \times \left(\sin\frac{\theta}{2}\right)^{2k+n-m} \left(\cos\frac{\theta}{2}\right)^{2\ell-2k-(n-m)}. \end{aligned} \tag{30}$$

Let $d\mu(g)$ denote the normalized invariant volume element on $SO(3)$, which is expressed, in terms of the Euler angles, as

$$d\mu(g) = \frac{1}{8\pi^2} \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi\, \mathrm{d}\psi \qquad \text{with} \quad \int_{SO(3)} d\mu(g) = 1. \tag{31}$$

According to equation (9) with $\rho_{ij}^\chi = D_{mn}^\ell$ and $d_\chi = 2\ell + 1$, etc., a wavefunction $f(hx)$ on M with $h \in SO(3)$ is expanded into a Fourier series

$$f(hx) = \sum_{\ell=0}^{\infty} \sum_{|m|,|n|\leqslant\ell} (2\ell+1) D_{mn}^\ell(h) \int_{SO(3)} \bar{D}_{mn}^\ell(g) f(gx)\, \mathrm{d}\mu(g) \qquad x \in M. \tag{32}$$

We can use equation (32) to write out $f(x)$ in terms of local coordinates in M. Let (r_1, r_2, φ) be internal coordinates, local coordinates in the orbit space $Q = M/SO(3)$, defined through

$$r_1 = |\boldsymbol{r}_1| \qquad r_2 = |\boldsymbol{r}_2| \qquad \boldsymbol{r}_1 \cdot \boldsymbol{r}_2 = r_1 r_2 \cos\varphi \tag{33}$$

which determines a local section $\sigma : V \subset Q \to M$ by

$$\sigma : (r_1, r_2, \varphi) \mapsto \sigma(q) = (r_1 \boldsymbol{e}_3, r_2\, \mathrm{e}^{\varphi \hat{e}_2} \boldsymbol{e}_3) \tag{34}$$

where V is some open subset of the shape space $Q = M/SO(3)$, and $q \in V$. Here we comment on the domain of σ. Originally, V must be an open subset of $\dot{Q}$, so that we have to impose the condition $\varphi \neq 0$, for example. However, we may extend V so as to include the boundary points with $\varphi = 0$. In spite of this extension, we are allowed to call V an open subset of Q. Then any point x in $\pi^{-1}(V)$ is expressed as $x = g\sigma(q) = (gr_1\boldsymbol{e}_3, gr_2\, \mathrm{e}^{\varphi\hat{e}_2}\boldsymbol{e}_3)$. By setting $h = g$ and $x = \sigma(q)$ in equation (32), we obtain

$$f(g\sigma(q)) = \sum_{\ell=0}^{\infty} (2\ell+1) \sum_{|m|,|n|\leqslant\ell} D^{\ell}_{mn}(g) \int_{SO(3)} \bar{D}^{\ell}_{mn}(k) f(k\sigma(q))\, \mathrm{d}\mu(k). \tag{35}$$

By using the operators P^{ℓ}_{nm} defined in the same manner as in equation (15), equation (35) is rewritten as

$$f(g\sigma(q)) = \sum_{\ell=0}^{\infty} \sum_{|m|,|n|\leqslant\ell} D^{\ell}_{mn}(g) \big(P^{\ell}_{nm} f\big)(\sigma(q)). \tag{36}$$

We may take another local section $\tau : W \to M$ with $W \cap V \neq \emptyset$. Then $x \in \pi^{-1}(V \cap W)$ has another expression, $x = h\tau(q)$. The right-hand side of equation (36) takes a slightly different form accordingly, but it is related to the original expression by a suitable transformation arising from equation (19).

The map $E^{\ell}_m : L^2(M) \to \mathcal{H}^{\ell} \otimes L^2(M)$ is defined as in equation (20)

$$E^{\ell}_m f = \frac{1}{\sqrt{2\ell+1}} \sum_{|m'|\leqslant\ell} e^{\ell}_{m'} \otimes P^{\ell}_{m'm} f \tag{37}$$

where $e^{\ell}_{m'}$, denoted usually by $|\ell m'\rangle$, is the basis of the representation space $\mathcal{H}^{\ell}$ assigned by ℓ. The ρ^{χ} equivariance condition (22) now takes the form

$$\big(E^{\ell}_m f\big)(hx) = D^{\ell}(h)\big(E^{\ell}_m f\big)(x). \tag{38}$$

Taking the local expression $x = g\sigma(q)$, we obtain $\big(E^{\ell}_m f\big)(x) = D^{\ell}(g)\big(E^{\ell}_m f\big)(\sigma(q))$, which shows that $\big(E^{\ell}_m f\big)(x)$ is a vector of eigenstates associated with the total angular momentum $\ell(\ell+1)$.

In general, from the D^{ℓ} equivariance condition (38), we can observe that the component function $P^{\ell}_{nm} f$ has the eigenvalue $-n$ associated with the projection of angular momentum on the $\boldsymbol{e}_3$-axis. In fact, for a rotation $\mathrm{e}^{t\hat{e}_3}$ around the $\boldsymbol{e}_3$-axis, we have

$$D^{\ell}_{nm}(\mathrm{e}^{t\hat{e}_3}) = \mathrm{e}^{-\mathrm{i}tn} \delta_{nm} \qquad t \in \mathbf{R} \tag{39}$$

and therefore, from the second equation of (19),

$$\big(P^{\ell}_{nm} f\big)(\mathrm{e}^{t\hat{e}_3} x) = \sum_{|m'|\leqslant\ell} D^{\ell}_{nm'}(\mathrm{e}^{t\hat{e}_3}) \big(P^{\ell}_{m'm} f\big)(x) = \mathrm{e}^{-\mathrm{i}nt} \big(P^{\ell}_{nm} f\big)(x). \tag{40}$$

Differentiating both sides of equation (40) with respect to t at $t = 0$, we obtain

$$\big(\hat{J}_3 P^{\ell}_{nm} f\big)(x) := \frac{1}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\big(P^{\ell}_{nm} f\big)(\mathrm{e}^{t\hat{e}_3}x)|_{t=0} = -n\big(P^{\ell}_{nm} f\big)(x) \tag{41}$$

where $\hat{J}_3$ is the projection of angular momentum operator on the $\boldsymbol{e}_3$-axis.

In contrast with this, if we use the first equation of (19), we will obtain, instead of equation (41),

$$P^{\ell}_{nm}\hat{J}_3 f = -m P^{\ell}_{nm} f. \tag{42}$$

5. Boundary conditions at collinear configurations

Here we consider the case where the three particles are aligned collinearly. We take the line on which the particles are aligned to be the $\boldsymbol{e}_3$-axis and set

$$\zeta_0 := \sigma(q_0) = (r_1\boldsymbol{e}_3, r_2\boldsymbol{e}_3) \tag{43}$$

where $q_0 = (r_1, r_2, 0)$ with $\varphi = 0$. Then the isotropy subgroup at $\zeta_0 \in M$ is given by $\mathrm{e}^{t\hat{e}_3}$. Hence, for a wavefunction f, we have

$$f(\mathrm{e}^{t\hat{e}_3}\zeta_0) = f(\zeta_0) \tag{44}$$

at the collinear configuration ζ_0. Differentiating this equation with respect to t at $t = 0$ results in

$$(\hat{J}_3 f)(\zeta_0) = 0 \tag{45}$$

which implies that, if $f(\zeta_0) \neq 0$, the projection of angular momentum on the axis of collinear configuration vanishes. By contraposition, this can be interpreted as follows. If the projection of angular momentum on an axis does not vanish, then three particles will not be aligned on the axis, i.e. the probability that the three particles happen to be aligned on the line is zero.

It is to be noted that we can choose any axis other than $\boldsymbol{e}_3$-axis as the one on which three particles are aligned. In fact, if we take $\boldsymbol{e}'_3 = h\boldsymbol{e}_3$, and set $\zeta'_0 = (r_1\boldsymbol{e}'_3, r_2\boldsymbol{e}'_3)$, then for the isotropy subgroup $\mathrm{e}^{t\hat{e}'_3}$ at ζ'_0, we have $f(\mathrm{e}^{t\hat{e}'_3}\zeta'_0) = f(\zeta'_0)$. From $\mathrm{e}^{t\hat{e}'_3} = h\mathrm{e}^{t\hat{e}_3}h^{-1}$, this equation becomes

$$f(\mathrm{e}^{t\hat{e}'_3}\zeta'_0) = (U(h)\mathrm{e}^{\mathrm{i}t\hat{J}_3}U(h^{-1})f)(\zeta'_0) = (\mathrm{e}^{\mathrm{i}t\hat{K}_3} f)(\zeta'_0) = f(\zeta'_0) \tag{46}$$

where $\hat{K}_3$ is one of the angular momentum operators with respect to the so-called body frame. When differentiated with respect to t at $t = 0$, the above equation provides

$$(\hat{K}_3 f)(\zeta'_0) = 0 \tag{47}$$

implying that if $f(\zeta'_0) \neq 0$, the projection of angular momentum on the $\boldsymbol{e}'_3$-axis vanishes.

The counterpart of this fact in classical mechanics is easy to see. Let $(\boldsymbol{r}_1(t), \boldsymbol{r}_2(t))$ be a trajectory of a classical three-body system. If the three bodies are aligned on a line at t_0, we have $\boldsymbol{r}_1(t_0) = \lambda_1\boldsymbol{d}$ and $\boldsymbol{r}_2(t_0) = \lambda_2\boldsymbol{d}$, where $\boldsymbol{d}$ is a unit vector in the line of alignment and $(\lambda_1, \lambda_2) \neq (0, 0)$ are constants. Then we have

$$(\boldsymbol{r}_1(t) \times \dot{\boldsymbol{r}}_1(t) + \boldsymbol{r}_2(t) \times \dot{\boldsymbol{r}}_2(t)) \cdot \boldsymbol{d} = (\boldsymbol{r}_1(t_0) \times \dot{\boldsymbol{r}}_1(t_0) + \boldsymbol{r}_2(t_0) \times \dot{\boldsymbol{r}}_2(t_0)) \cdot \boldsymbol{d} = 0 \tag{48}$$

which shows that the total angular momentum vanishes when projected on the axis on which three bodies are aligned. It then follows by contraposition that if the angular momentum has a non-vanishing component around $\boldsymbol{d}$, three particles will not be aligned on the $\boldsymbol{d}$-axis.

So far we have obtained the physically reasonable boundary condition at the singular configuration ζ_0. Referring to the Fourier series expansion (36) and the equivariance condition (38), we can obtain the same boundary condition. Since the isotropy subgroup is represented as in equation (39), the equivariance condition at ζ_0 takes the form

$$\big(P^{\ell}_{nm}f\big)(\zeta_0)=\mathrm{e}^{-\mathrm{i}nt}\big(P^{\ell}_{nm}f\big)(\zeta_0) \tag{49}$$

which implies that

$$\big(P^{\ell}_{nm}f\big)(\zeta_0)=0 \qquad \text{if} \quad n\neq 0. \tag{50}$$

Since $-n$ assigns an angular momentum eigenvalue (see equation (41)), we verify again that if the angular momentum n is not zero, the wavefunction must vanish at ζ_0.

We now wish to gain an insight into the behaviour of the wavefunction $f(g\sigma(q))$ around the collinear configuration ζ_0 in more detail. Setting $g=\mathrm{e}^{\phi\hat{e}_3}\mathrm{e}^{\theta\hat{e}_2}\mathrm{e}^{\psi\hat{e}_3}=g_0\,\mathrm{e}^{\psi\hat{e}_3}$ with $g_0=\mathrm{e}^{\phi\hat{e}_3}\mathrm{e}^{\theta\hat{e}_2}$, we put $f(g\sigma(q))$ in the form $f\big(g_0\mathrm{e}^{\psi\hat{e}_3}\sigma(q)\big)$. It is to be noted that when q tends to q_0 (i.e. $\varphi\to 0$), $g_0\mathrm{e}^{\psi\hat{e}_3}\sigma(q)$ approaches $g_0\sigma(q_0)$ on account of $\mathrm{e}^{\psi\hat{e}_3}\sigma(q_0)=\sigma(q_0)$. In view of this, we break up the set of local coordinates into two: (θ,ϕ) and (ψ,r_1,r_2,φ). The coordinates (θ,ϕ) becomes those for describing the orbit $\mathcal{O}_{q_0}$ when $\varphi=0$. Furthermore, in place of (ψ,r_1,r_2,φ), we introduce new local coordinates (r_1,ξ_1,ξ_2,ξ_3) by

$$\xi_1=r_2\sin\varphi\cos\psi \qquad \xi_2=r_2\sin\varphi\sin\psi \qquad \xi_3=r_2\cos\varphi. \tag{51}$$

Then the configuration $\mathrm{e}^{\psi\hat{e}_3}\sigma(q)$ is put in the form

$$\mathrm{e}^{\psi\hat{e}_3}\sigma(q)=(r_1\boldsymbol{e}_3,\xi_1\boldsymbol{e}_1+\xi_2\boldsymbol{e}_2+\xi_3\boldsymbol{e}_3). \tag{52}$$

To look into a geometric meaning of the new coordinates, we consider the tangent space $T_{\sigma(q_0)}(M)$ at the collinear configuration $\sigma(q_0)=(r_1\boldsymbol{e}_3,r_2\boldsymbol{e}_3)$. We note that the tangent space to the orbit $\mathcal{O}_{\sigma(q_0)}$ is described as

$$T_{\sigma(q_0)}\big(\mathcal{O}_{\sigma(q_0)}\big)=\mathrm{span}\{(r_1\boldsymbol{e}_1,r_2\boldsymbol{e}_1),(r_1\boldsymbol{e}_2,r_2\boldsymbol{e}_2)\}. \tag{53}$$

We now take the subspace $V_{\sigma(q_0)}$ of $T_{\sigma(q_0)}(M)$ that is given by

$$V_{\sigma(q_0)}=\mathrm{span}\{(\boldsymbol{e}_3,0),(0,\boldsymbol{e}_3),(0,\boldsymbol{e}_1),(0,\boldsymbol{e}_2)\}. \tag{54}$$

Then we have the direct sum decomposition of $T_{\sigma(q_0)}(M)$,

$$T_{\sigma(q_0)}(M)=T_{\sigma(q_0)}(\mathcal{O}_{\sigma(q_0)})\oplus V_{\sigma(q_0)}. \tag{55}$$

Although the subspace $V_{\sigma(q_0)}$ is not orthogonal to $T_{\sigma(q_0)}(\mathcal{O}_{\sigma(q_0)})$ with respect to the canonical metric $\mathrm{d}s^2=\sum \mathrm{d}\boldsymbol{r}_k\cdot\mathrm{d}\boldsymbol{r}_k$, its basis vectors are capable of geometric interpretation. The vectors $(\boldsymbol{e}_3,0)$, $(0,\boldsymbol{e}_3)$ correspond to the differential operators $\partial/\partial r_1$, $\partial/\partial\xi_3$ at $\sigma(q_0)$, respectively, and $(0,\boldsymbol{e}_1)$, $(0,\boldsymbol{e}_2)$ to $\partial/\partial\xi_1$, $\partial/\partial\xi_2$ at $\sigma(q_0)$, respectively. If the tangent vectors $(\boldsymbol{e}_3,0)$, $(0,\boldsymbol{e}_3)$ are applied to deform infinitesimally the configuration $\sigma(q_0)$, it remains collinear. In contrast with this, if the tangent vectors $(0,\boldsymbol{e}_1)$, $(0,\boldsymbol{e}_2)$ are applied, the configuration $\sigma(q_0)$ becomes bent. Thus we are convinced that the coordinates (ξ_1,ξ_2) play a specific role in the study of boundary behaviour of wavefunctions at collinear configurations. Note also that collinear configurations are assigned by the condition $\xi_1=\xi_2=0$.

We further set

$$z=\xi_1+\mathrm{i}\xi_2=\rho\mathrm{e}^{\mathrm{i}\psi} \qquad \rho=r_2\sin\varphi \tag{56}$$

where ρ is a shape parameter expressed also as

$$\rho=\|\boldsymbol{r}_1\times\boldsymbol{r}_2\|/r_1. \tag{57}$$

The coordinates (ρ,ψ) play a specific role, like (ξ_1,ξ_2).

If we view the wavefunction $f\big(g_0\mathrm{e}^{\psi\hat{e}_3}\sigma(q)\big)$ as a function of ψ, we may put equation (36) in the form of a Fourier series expansion with respect to ψ

$$f(g_0\mathrm{e}^{\psi\hat{e}_3}\sigma(q))=\sum_{n=-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}n\psi}\sum_{\ell\geqslant|n|}^{\infty}\sum_{|m|\leqslant\ell}\mathrm{e}^{-\mathrm{i}m\phi}d^{\ell}_{mn}(\theta)\big(P^{\ell}_{nm}f\big)(\sigma(q)) \tag{58}$$

which is, of course, written as

$$f(g_0 \mathrm{e}^{\psi \hat{e}_3} \sigma(q)) = \sum_{n=-\infty}^{\infty} c_n(g_0; r_1, r_2, \varphi)\, \mathrm{e}^{\mathrm{i}n\psi} \tag{59}$$

where

$$c_n(g_0; r_1, r_2, \varphi) := \frac{1}{2\pi} \int_0^{2\pi} \mathrm{e}^{-\mathrm{i}n\psi} f(g_0\, \mathrm{e}^{\psi \hat{e}_3} \sigma(q))\, \mathrm{d}\psi. \tag{60}$$

We assume here that the function $f\big(g_0; \mathrm{e}^{\psi \hat{e}_3} \sigma(q)\big) = f(g_0; r_1, \xi_1, \xi_2, \xi_3)$ is analytic in ξ_1, ξ_2, which is the case if $f(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is analytic in $\boldsymbol{r}_2$. Then it may be expanded into a power series in $z, \overline{z}$ and expressed as

$$\begin{aligned} f(g_0\, \mathrm{e}^{\psi \hat{e}_3} \sigma(q)) &= \sum_{\ell, m \geqslant 0}^{\infty} c_{\ell m}(g_0; r_1, \xi_3) z^{\ell} \overline{z}^{m} \\ &= \sum_{\ell, m \geqslant 0}^{\infty} c_{\ell m}(g_0; r_1, \xi_3) \rho^{\ell + m} \mathrm{e}^{\mathrm{i}(\ell - m)\psi} \\ &= \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}n\psi} \sum_{k=0}^{\infty} \rho^{|n|+2k} C_{kn}(g_0; r_1, \xi_3) \end{aligned} \tag{61}$$

where

$$C_{kn} = c_{k+\frac{1}{2}(|n|+n), k+\frac{1}{2}(|n|-n)}. \tag{62}$$

Thus, we have obtained the Fourier coefficient $c_n(g_0; r_1, r_2, \varphi)$ expressed as

$$c_n(g_0; r_1, r_2, \varphi) = \sum_{k=0}^{\infty} \rho^{|n|+2k} C_{kn}(g_0; r_1, \xi_3). \tag{63}$$

Proposition 1. *If a wavefunction f is analytic in the neighbourhood of the collinear configuration, the Fourier coefficient $c_n(g_0; r_1, r_2, \varphi)$ with respect to the rotation around the axis of alignment is expressed as a power series of ρ which starts with a term of the lowest order $|n|$ and contains every other integer power only, where n is the eigenvalue of the projection of angular momentum operator on the axis of alignment, and $\rho = \|\boldsymbol{r}_1 \times \boldsymbol{r}_2\|/r_1$ describes how the shape formed by the three bodies is distant from a collinear shape.*

This proposition implies that the larger the projection of angular momentum, $|n|$, on an axis becomes, the less the three bodies are likely to be aligned on the axis. If we let $\sigma(q) \to \sigma(q_0)$, i.e. $\varphi \to 0$ or π, then we have $\xi_3 = r_2 \cos\varphi \to r_2$ and $\rho = r_2 \sin\varphi \to 0$, so that the right-hand side of equation (63) vanish if $n \neq 0$. Thus, we have found again that if the projection of angular momentum on the axis of alignment does not vanish, the wavefunction must vanish at the collinear configuration.

We also have to notice that proposition 1 holds true independently of the choice of an axis of alignment. If we want to choose $\boldsymbol{e}_3' = h\boldsymbol{e}_3$, $h \in SO(3)$, as the axis of alignment, we can take a local section

$$\sigma'(q) = \big(r_1 \boldsymbol{e}_3', r_2\, \mathrm{e}^{\varphi \hat{e}_2'} \boldsymbol{e}_3'\big) = h\sigma(q) \tag{64}$$

where $\boldsymbol{e}_2' = h\boldsymbol{e}_2$. We denote the rotation matrix by $g' = \mathrm{e}^{\phi \hat{e}_3'} \mathrm{e}^{\theta \hat{e}_2'} \mathrm{e}^{\psi \hat{e}_3'}$. Then we have

$$g'\sigma'(q) = g_0'\, \mathrm{e}^{\psi \hat{e}_3'} \sigma'(q) = h g_0 \mathrm{e}^{\psi \hat{e}_3} \sigma(q) \tag{65}$$

where $g_0' = e^{\phi\hat{e}_3'}e^{\theta\hat{e}_2'}$, so that the Fourier coefficient $c_n'(g_0'; r_1, r_2, \varphi)$ with respect to the rotation around the $\boldsymbol{e}_3'$-axis should be expressed as $c_n(hg_0; r_1, r_2, \varphi)$ and have the same power series expansion as equation (63) in ρ.

We have to point out in conclusion of this section that proposition 1 was first proved by Mitchell and Littlejohn in quite a different manner [9]. In addition, we notice that the boundary behaviour of wavefunctions around the collinear configurations plays a significant role in showing that the singularity the kinetic energy operator has at the collinear configurations is not essential in the sense that the kinetic energy integral is not divergent at the collinear configurations (see [13]).

6. Boundary conditions at triple collision

In this section, we wish to consider how wavefunctions behave in the neighbourhood of the triple collision. The equivariance condition (38) at $0 \in M_0$ takes the form

$$\big(E_m^\ell f\big)(0) = D^\ell(h)\big(E_m^\ell f\big)(0) \qquad h \in SO(3). \tag{66}$$

From this it follows that if $\big(E_m^\ell f\big)(0) \neq 0$, we have a non-trivial invariant subspace of the representation space $\mathcal{H}^\ell$. If $\ell \neq 0$, this would contradict the fact that D^ℓ are irreducible representations. Thus we obtain $\big(E_m^\ell f\big)(0) = 0$ for $\ell \neq 0$, or

$$\big(P_{nm}^\ell f\big)(0) = 0 \qquad \text{if} \quad \ell \neq 0. \tag{67}$$

This implies that if the total angular momentum does not vanish, the triple collision will not take place. If $\ell = 0$, then the representation space is one-dimensional, so that $\big(E_0^0 f\big)(0)$ may take a non-zero value. Hence, the triple collision may take place, if $\ell = 0$.

The counterpart of this fact in classical mechanics is easy to describe. If the triple collision may take place, we have $\boldsymbol{r}_1(t_0) = \boldsymbol{r}_2(t_0) = 0$ at a certain time t_0, so that

$$\boldsymbol{r}_1 \times \dot{\boldsymbol{r}}_1 + \boldsymbol{r}_2 \times \dot{\boldsymbol{r}}_2 = 0 \tag{68}$$

for all time on account of the conservation of the total angular momentum. By contraposition, if the total angular momentum does not vanish, then the triple collision cannot take place.

We proceed to study the boundary behaviour of wavefunctions at the triple collision in more detail. Our objective is to extend proposition 1 to the case of triple collision. We identify the centre-of-mass system M with $\mathbf{R}^3 \times \mathbf{R}^3$ and denote the Cartesian coordinates of $\mathbf{R}^3 \times \mathbf{R}^3$ by (ξ_i, η_j), $i, j = 1, 2, 3$. For notational convenience, we use $\boldsymbol{\xi}, \boldsymbol{\eta}$ for $\boldsymbol{r}_1, \boldsymbol{r}_2$. We assume that a wavefunction $f(\boldsymbol{\xi}, \boldsymbol{\eta})$ on $\mathbf{R}^3 \times \mathbf{R}^3$ is analytic at the origin. Then, f has the expansion of the form

$$f(\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{I,J} c_{IJ}\xi^I \eta^J \tag{69}$$

where

$$I = (i_1, i_2, i_3) \qquad J = (j_1, j_2, j_3) \qquad \xi^I = \xi_1^{i_1}\xi_2^{i_2}\xi_3^{i_3} \qquad \eta^J = \eta_1^{j_1}\eta_2^{j_2}\eta_3^{j_3}. \tag{70}$$

We wish to bring this power series into a Fourier series like equation (36). To this end, we first break up equation (69) into the sum of homogeneous polynomials. Let $P^n(\mathbf{R}^3 \times \mathbf{R}^3)$ denote the space of homogeneous polynomials of degree n in ξ_i, η_j. It is a representation space for $SO(3)$ and will be decomposed into irreducible subspaces with respect to the $SO(3)$ action. In each irreducible subspace of dimension $2\ell + 1$, basis polynomials p_m will transform according to

$$p_m(g^{-1}\boldsymbol{\xi}, g^{-1}\boldsymbol{\eta}) = \sum_{|m'|\leqslant\ell} p_{m'}(\boldsymbol{\xi}, \boldsymbol{\eta})D_{m'm}^\ell(g). \tag{71}$$

The decomposition of $P^n(\mathbf{R}^3 \times \mathbf{R}^3)$ will be carried out as follows. Let $P^n(\mathbf{R}^3)$ denote the space of homogeneous polynomials in x_i, where x_i are the Cartesian coordinates of $\mathbf{R}^3$. Then, as is well known, $P^n(\mathbf{R}^3)$ is decomposed into

$$P^n(\mathbf{R}^3) = H^n(\mathbf{R}^3) \oplus r^2 H^{n-2}(\mathbf{R}^3) \oplus \cdots \oplus \begin{cases} r^n H^0(\mathbf{R}^3) & \text{(if } n \text{ is even)} \\ r^{n-1} H^1(\mathbf{R}^3) & \text{(if } n \text{ is odd)} \end{cases} \tag{72}$$

where $r^2 = \sum_{i=1}^3 x_i^2$ and $H^m(\mathbf{R}^3)$ is the space of solid harmonics of degree m. As is well known, $H^m(\mathbf{R}^3)$ is isomorphic with the $(2m+1)$-dimensional space V_m for unitary irreducible representations of $SO(3)$. Since r^2 is invariant under the $SO(3)$ action, the above decomposition implies that

$$P^n(\mathbf{R}^3) \cong V_n \oplus V_{n-2} \oplus \cdots \oplus \begin{cases} V_0 & \text{(if } n \text{ is even)} \\ V_1 & \text{(if } n \text{ is odd)} \end{cases}. \tag{73}$$

We here notice that

$$P^k\big(\mathbf{R}^3 \times \mathbf{R}^3\big) = \sum_{n+m=k} P^n(\mathbf{R}^3) \otimes P^m(\mathbf{R}^3). \tag{74}$$

Equations (72) and (74) are put together to yield

$$\begin{aligned} P^k\big(\mathbf{R}^3_\xi \times \mathbf{R}^3_\eta\big) = &\sum_{n+m=k} H^n\big(\mathbf{R}^3_\xi\big) \otimes H^m\big(\mathbf{R}^3_\eta\big) \oplus \sum_{n+m=k, m\geqslant 2} H^n\big(\mathbf{R}^3_\xi\big) \otimes |\boldsymbol{\eta}|^2 H^{m-2}\big(\mathbf{R}^3_\eta\big) \\ &\oplus \sum_{n+m=k, n\geqslant 2} |\boldsymbol{\xi}|^2 H^{n-2}\big(\mathbf{R}^3_\xi\big) \otimes H^m\big(\mathbf{R}^3_\eta\big) \oplus \cdots. \end{aligned} \tag{75}$$

This decomposition gives rise to the following isomorphism

$$P^k(\mathbf{R}^3 \times \mathbf{R}^3) \cong \sum_{n+m=k} V_n \otimes V_m \oplus \sum_{n+m=k, m\geqslant 2} V_n \otimes V_{m-2} \oplus \sum_{n+m=k, n\geqslant 2} V_{n-2} \otimes V_m \oplus \cdots. \tag{76}$$

We here apply the Clebsch–Gordan decomposition formula for tensor product representations of $SO(3)$ [14]

$$V_p \otimes V_q \cong V_{|p-q|} \oplus V_{|p-q|+1} \oplus \cdots \oplus V_{p+q} \tag{77}$$

to the right-hand side of equation (76) to obtain

$$P^k(\mathbf{R}^3 \times \mathbf{R}^3) \cong (k+1)V_k \oplus (k-1)V_{k-1} \oplus \cdots \tag{78}$$

where we have to note that $(k+1)V_k$ in the right-hand side of equation (78) denotes $k+1$ representation spaces isomorphic to one another. The multiple occurrence of V_m in the decomposition of $P^k(\mathbf{R}^3 \times \mathbf{R}^3)$ implies that there are a variety of realizations of V_m as spaces of homogeneous polynomials of the same degree k but of different types, so that we have a variety of basis polynomials that transform according to the same rule but have different realizations. Examples will be given in the next section. Equation (78) means that $P^k(\mathbf{R}^3 \times \mathbf{R}^3)$ includes representation spaces V_m with $m \leqslant k$ only. Then we obtain the following.

Lemma 2. *If all the spaces of homogeneous polynomials are decomposed into unitary irreducible representation spaces of $SO(3)$, the representation space V_ℓ arises from $P^k(\mathbf{R}^3 \times \mathbf{R}^3)$ with $k \geqslant \ell$.*

We are now in a position to bring the Taylor series (69) into a Fourier series with respect to D functions. For an open subset U of the orbit space Q, there exists a local section $\sigma : U \to M$.

Then we can express any point $(\boldsymbol{\xi}, \boldsymbol{\eta}) \in \pi^{-1}(U)$ as

$$(\boldsymbol{\xi}, \boldsymbol{\eta}) = (g\boldsymbol{\sigma}_1(q), g\boldsymbol{\sigma}_2(q)) \qquad g \in SO(3) \qquad q \in U. \tag{79}$$

If we decompose each homogeneous part of equation (69), $\sum_{|I|+|J|=k} c_{IJ}\xi^I\eta^J$ with $|I| = i_1 + i_2 + i_3$ and $|J| = j_1 + j_2 + j_3$, into a linear combination of basis polynomials according to equation (78), and arrange the terms with respect to the representation spaces V_ℓ, then equation (69) is put in the form

$$f(\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{\ell=0}^{\infty} f_\ell(\boldsymbol{\xi}, \boldsymbol{\eta}) \qquad f_\ell(\boldsymbol{\xi}, \boldsymbol{\eta}) := \sum_{n \geqslant \ell} p^{(\ell,n)}(\boldsymbol{\xi}, \boldsymbol{\eta}) \tag{80}$$

where $p^{(\ell,n)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ denotes a linear combination of all basis polynomials of degree $n(\geqslant \ell)$ that are in $\mu_{\ell,n}V_\ell$, where $\mu_{\ell,n}$ is the multiplicity of V_ℓ in the decomposition of $P^n(\mathbf{R}^3 \times \mathbf{R}^3)$:

$$p^{(\ell,n)}(\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{|m| \leqslant \ell} a_m^{(\ell,n)} p_m^{(\ell,n)}(\boldsymbol{\xi}, \boldsymbol{\eta}) + \cdots \quad \text{(the sum of } \mu_{\ell,n} \text{ similar terms)}. \tag{81}$$

We now insert the coordinate description (79) of $(\boldsymbol{\xi}, \boldsymbol{\eta})$ into $p^{(\ell,n)}(\boldsymbol{\xi}, \boldsymbol{\eta})$, and use the transformation rule (71) for basis polynomials. Then we can put $f_\ell(\boldsymbol{\xi}, \boldsymbol{\eta})$ in the form

$$f_\ell(\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{n \geqslant \ell} p^{(\ell,n)}(g\boldsymbol{\sigma}_1(q), g\boldsymbol{\sigma}_2(q)) = \sum_{|m|,|m'| \leqslant \ell} D^\ell_{mm'}(g^{-1}) c^{(\ell)}_{mm'}(q) \tag{82}$$

where

$$c^{(\ell)}_{mm'}(q) = \sum_{n \geqslant \ell} a_m^{(\ell,n)} p_{m'}^{(\ell,n)}(\boldsymbol{\sigma}_1(q), \boldsymbol{\sigma}_2(q)) + \cdots. \tag{83}$$

Thus, the power series (69) is put in the form of a Fourier series with respect to D functions:

$$f(g\boldsymbol{\sigma}_1(q), g\boldsymbol{\sigma}_2(q)) = \sum_{\ell=0}^{\infty} \sum_{|m|,|m'| \leqslant \ell} D^\ell_{mm'}(g^{-1}) c^{(\ell)}_{mm'}(q). \tag{84}$$

Summing up the above, we obtain the following.

Proposition 3. *Suppose that a wavefunction f for a three-body system is analytic at the origin of the centre-of-mass system $\mathbf{R}^3 \times \mathbf{R}^3$. Then f can be decomposed into the sum of eigenstates f_ℓ associated with the eigenvalue $\ell(\ell + 1)$ of the total angular momentum operator (see equations (80) and (82)). The eigenstate f_ℓ is expressed as a power series in ξ_i, η_j, which starts with the lowest-order terms of the form $\xi^I\eta^J$ with $|I| + |J| = \ell$, where $|I| = i_1 + i_2 + i_3$, $|J| = j_1 + j_2 + j_3$. Furthermore, f_ℓ can be expressed as a linear combination of $D^\ell_{mn}(g)$ with $|n|, |m| \leqslant \ell$, coefficients of which are functions of shape variables (see equation (83)).*

This proposition implies that the more the total angular momentum $\ell(\ell+1)$ grows, the less the three particles are likely to collide simultaneously. We notice in addition that boundary conditions at the triple collision for a planar three-body system have been obtained in [15], which looks rather like proposition 1. In conclusion, we notice that our result is independent of the Hamiltonian operator. In [13], it is shown also that the singularity the kinetic energy operator has at the triple collision is not essential in the sense that the kinetic energy integral is not divergent at the triple collision. If the Hamiltonian operator is of the harmonic oscillator type, the boundary behaviour of wavefunctions at the origin (i.e. at the triple collision) are already known (see [16], for instance).

7. Remarks

In conclusion, in order to obtain examples of basis polynomials transforming as equation (71), we work with the Clebsch–Gordan decomposition formula (77) in the cases of $p = q = 1$ and of $p = 2, q = 1$ in detail. First we take the case of $p = q = 1$. For $V_1 \cong H^1(\mathbf{R}^3_\xi)$ and $V_1 \cong H^1(\mathbf{R}^3_\eta)$, we have

$$H^1(\mathbf{R}^3_\xi) \otimes H^1(\mathbf{R}^3_\eta) \cong V_0 \oplus V_1 \oplus V_2. \tag{85}$$

We will study how $V_\ell, \ell = 0, 1, 2$, are realized as spaces of polynomials in $\boldsymbol{\xi}, \boldsymbol{\eta}$. It is easy to see that a basis polynomial in V_0 is given by

$$p^{(0)}(\boldsymbol{\xi}, \boldsymbol{\eta}) = \boldsymbol{\xi} \cdot \boldsymbol{\eta}. \tag{86}$$

This is because it is invariant under the $SO(3)$ action.

We turn to V_1. Let

$$\boldsymbol{\zeta} = \boldsymbol{\xi} \times \boldsymbol{\eta}. \tag{87}$$

Then, under the $SO(3)$ action, $\boldsymbol{\zeta}$ transforms according to $\boldsymbol{\zeta} \mapsto g\boldsymbol{\zeta}$. As is well known [12], the polynomials defined to be

$$\left(q_1^{(1)}(\boldsymbol{x}), q_0^{(1)}(\boldsymbol{x}), q_{-1}^{(1)}(\boldsymbol{x})\right) = \left(-\frac{x_1 + \mathrm{i}x_2}{\sqrt{2}}, x_3, \frac{x_1 - \mathrm{i}x_2}{\sqrt{2}}\right) \tag{88}$$

transform according to

$$q_n^{(1)}(g^{-1}\boldsymbol{x}) = \sum_{|m|\leqslant 1} q_m^{(1)}(\boldsymbol{x}) D^1_{mn}(g). \tag{89}$$

In fact, the polynomials $q_m^{(1)}(\boldsymbol{x})$ are related to the spherical harmonics by

$$q_m^{(1)}(\boldsymbol{x}) = \sqrt{\frac{4\pi}{3}} r Y_{1m}(\theta, \phi) \qquad m = 1, 0, -1. \tag{90}$$

Thus, we have found the following basis polynomials in V_1:

$$p_m^{(1)}(\boldsymbol{\xi}, \boldsymbol{\eta}) := q_m^{(1)}(\boldsymbol{\xi} \times \boldsymbol{\eta}) \qquad m = -1, 0, 1. \tag{91}$$

Before proceeding to V_2, we notice that

$$H^1(\mathbf{R}^3_\xi) \otimes H^1(\mathbf{R}^3_\eta) = \{\mathrm{tr}(C\boldsymbol{\xi}\boldsymbol{\eta}^T) | C \in \mathbf{C}^{3\times 3}\} \tag{92}$$

where $\mathbf{C}^{3\times 3}$ denotes the vector space of the 3×3 complex matrices, which is endowed with the inner product through $\langle C_1, C_2\rangle = \mathrm{tr}(C_1^* C_2)$ with C^* denoting the Hermitian conjugate of C. The right-hand side of equation (92) may be identified with $\mathbf{C}^{3\times 3}$. The $SO(3)$ action $(\boldsymbol{\xi}, \boldsymbol{\eta}) \mapsto (g^{-1}\boldsymbol{\xi}, g^{-1}\boldsymbol{\eta})$ gives rise to a unitary transformation on $\mathbf{C}^{3\times 3}$ in the manner

$$C \longmapsto gCg^{-1} \qquad g \in SO(3). \tag{93}$$

As is easily seen, $\mathbf{C}^{3\times 3}$ is decomposed into the orthogonal direct sum

$$\mathbf{C}^{3\times 3} = M_0(3, \mathbf{C}) \oplus M_1(3, \mathbf{C}) \oplus M_2(3, \mathbf{C}) \tag{94}$$

where

$$M_0(3, \mathbf{C}) = \{\lambda I_3 | \lambda \in \mathbf{C}\} \tag{95}$$

$$M_1(3, \mathbf{C}) = \{C \in \mathbf{C}^{3\times 3} | C = -C^T\} \tag{96}$$

$$M_2(3, \mathbf{C}) = \{C \in \mathbf{C}^{3\times 3} | C = C^T, \mathrm{tr}(C) = 0\}. \tag{97}$$

This may be viewed as a realization of the Clebsch–Gordan decomposition, $\mathbf{C}^{3\times 3} = \mathbf{C}^3 \otimes \mathbf{C}^3 \cong V_0 \oplus V_1 \oplus V_2$. Put another way, $M_0(3, \mathbf{C})$, $M_1(3, \mathbf{C})$, $M_2(3, \mathbf{C})$ are realizations of V_0, V_1, V_2, respectively. The basis polynomials we have already found are associated with bases of $M_0(3, \mathbf{C})$ and of $M_1(3, \mathbf{C})$

$$p^{(0)}(\boldsymbol{\xi}, \boldsymbol{\eta}) = \mathrm{tr}(I_3 \boldsymbol{\xi}\boldsymbol{\eta}^T) \qquad p_m^{(1)}(\boldsymbol{\xi}, \boldsymbol{\eta}) = \mathrm{tr}(\gamma_m \boldsymbol{\xi}\boldsymbol{\eta}^T) \qquad |m| \leqslant 1 \tag{98}$$

where

$$\gamma_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 1 \\ \mathrm{i} & -1 & 0 \end{pmatrix} \qquad \gamma_0 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \gamma_{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & -1 \\ \mathrm{i} & 1 & 0 \end{pmatrix}. \tag{99}$$

We now discuss the realization of V_2 in terms of polynomials in $\boldsymbol{\xi}, \boldsymbol{\eta}$. Defining the following matrices, which are in $M_2(3, \mathbf{C})$,

$$\sigma_{-2} = \frac{1}{2}\begin{pmatrix} 1 & -\mathrm{i} & 0 \\ -\mathrm{i} & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \sigma_{-1} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & -\mathrm{i} \\ 1 & -\mathrm{i} & 0 \end{pmatrix} \qquad \sigma_0 = \frac{1}{\sqrt{6}}\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

$$\sigma_1 = \frac{1}{2}\begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\mathrm{i} \\ -1 & -\mathrm{i} & 0 \end{pmatrix} \qquad \sigma_2 = \frac{1}{2}\begin{pmatrix} 1 & \mathrm{i} & 0 \\ \mathrm{i} & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{100}$$

we set

$$p_m^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta}) = \mathrm{tr}(\sigma_m \boldsymbol{\xi}\boldsymbol{\eta}^T) \qquad |m| \leqslant 2. \tag{101}$$

Hence, the space $\mathrm{span}\{p_m^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta})\}_{|m|\leqslant 2}$ is a realization of the representation space V_2. We notice here that for $\boldsymbol{\xi} = \boldsymbol{\eta} = \boldsymbol{x}$, $p_m^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ reduce to the spherical harmonics

$$q_m^{(2)}(\boldsymbol{x}) := p_m^{(2)}(\boldsymbol{x}, \boldsymbol{x}) = \sqrt{\frac{8\pi}{15}} r^2 Y_{2m}(\theta, \phi) \tag{102}$$

which transform according to $q_m^{(2)}(g^{-1}\boldsymbol{x}) = \sum_{|n|\leqslant 2} q_n^{(2)}(\boldsymbol{x}) D_{nm}^2(g)$. Since the representation is unique up to equivalence, it turns out that $p_m^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ are subject to the same transformation as that for $q_m^{(2)}(\boldsymbol{x}) = p_m^{(2)}(\boldsymbol{x}, \boldsymbol{x})$:

$$p_m^{(2)}(g^{-1}\boldsymbol{\xi}, g^{-1}\boldsymbol{\eta}) = \sum_{|n|\leqslant 2} p_n^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta}) D_{nm}^2(g). \tag{103}$$

We consider the case of $p = 2, q = 1$. For $V_2 \cong H^2(\mathbf{R}_\xi^3)$ and $V_1 \cong H^1(\mathbf{R}_\eta^3)$, the Clebsch–Gordan formula gives

$$H^2(\mathbf{R}_\xi^3) \otimes H^1(\mathbf{R}_\eta^3) \cong V_1 \oplus V_2 \oplus V_3. \tag{104}$$

Basis polynomials in V_1 and in V_2 are given by

$$u_n^{(1)}(\boldsymbol{\xi}, \boldsymbol{\eta}) := \langle \boldsymbol{\xi}, \boldsymbol{\eta}\rangle q_n^{(1)}(\boldsymbol{\xi}) - \tfrac{1}{3}\langle \boldsymbol{\xi}, \boldsymbol{\xi}\rangle q_n^{(1)}(\boldsymbol{\eta}) \qquad |n| \leqslant 1 \tag{105}$$

$$u_m^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta}) := p_m^{(2)}(\boldsymbol{\xi} \times \boldsymbol{\eta}, \boldsymbol{\xi}) \qquad |m| \leqslant 2 \tag{106}$$

respectively, where $q_n^{(1)}(\boldsymbol{x})$ and $p_m^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ are given by equations (88) and (101), respectively. It is easy to verify that functions $u_n^{(1)}(\boldsymbol{\xi}, \boldsymbol{\eta})$, $u_m^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ are in $H^2(\mathbf{R}_\xi^3) \otimes H^1(\mathbf{R}_\eta^3)$ and transform in a satisfactory manner, respectively.

We proceed to basis polynomials in V_3. Let

$$Q_2(\boldsymbol{x}, t) := \sum_{|m|\leqslant 2} c_m^{(2)} q_m^{(2)}(\boldsymbol{x}) t^{2-m} \tag{107}$$

$$Q_1(\boldsymbol{x}, t) := \sum_{|n|\leqslant 1} c_n^{(1)} q_n^{(1)}(\boldsymbol{x}) t^{1-n} \tag{108}$$

where $q_m^{(2)}(\boldsymbol{x})$ and $q_n^{(1)}(\boldsymbol{x})$ are given by equations (102) and (88), respectively, and

$$\left(c_m^{(2)}\right) = (2, 4, 2\sqrt{6}, 4, 2) \qquad \left(c_n^{(1)}\right) = (\sqrt{2}, 2, \sqrt{2}). \tag{109}$$

We then define polynomials $p_k^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ through

$$Q_2(\boldsymbol{\xi}, t) Q_1(\boldsymbol{\eta}, t) = \sum_{|k|\leqslant 3} c_k^{(3)} p_k^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta}) t^{3-k} \tag{110}$$

where

$$\left(c_k^{(3)}\right) = (2\sqrt{6}, 12, 6\sqrt{10}, 4\sqrt{30}, 6\sqrt{10}, 12, 2\sqrt{6}). \tag{111}$$

It is easy to see that $p_k^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta}) \in H^2\left(\mathbf{R}^3_\xi\right) \otimes H^1\left(\mathbf{R}^3_\eta\right)$. To show that $p_k^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ are in V_3, we put the polynomials $u_n^{(1)}, u_m^{(2)}, p_k^{(3)}$ in the form $\mathrm{tr}(C^T P(\boldsymbol{\xi}, \boldsymbol{\eta}))$, where $C \in \mathbf{C}^{5\times 3}$, the space of 5×3 complex matrices, and $P(\boldsymbol{\xi}, \boldsymbol{\eta}) := \left(q_m^{(2)}(\boldsymbol{\xi}) q_n^{(1)}(\boldsymbol{\eta})\right) \in \mathbf{C}^{5\times 3}$ with $|m| \leqslant 3, |n| \leqslant 1$. Let $C_n^{(1)}, C_m^{(2)}, C_k^{(3)}$ denote the matrices associated with the polynomials $u_n^{(1)}, u_m^{(2)}, p_k^{(3)}$, respectively. Then, a straightforward calculation yields

$$C_{-1}^{(1)} = \begin{pmatrix} & & -1 \\ & \frac{\sqrt{2}}{2} & \\ -\frac{\sqrt{6}}{6} & & \\ 0 & & \\ 0 & & 0 \end{pmatrix} \qquad C_{0}^{(1)} = \begin{pmatrix} 0 & & 0 \\ & & -\frac{\sqrt{2}}{2} \\ & \frac{\sqrt{6}}{3} & \\ -\frac{\sqrt{2}}{2} & & \\ 0 & & 0 \end{pmatrix} \qquad C_{1}^{(1)} = \begin{pmatrix} 0 & & 0 \\ & & 0 \\ & & -\frac{\sqrt{6}}{6} \\ & \frac{\sqrt{2}}{2} & \\ -1 & & \end{pmatrix}$$

$$C_{-2}^{(2)} = \begin{pmatrix} & \mathrm{i} & 0 \\ -\frac{\sqrt{2}\mathrm{i}}{2} & & \\ 0 & & \\ 0 & & \\ 0 & & 0 \end{pmatrix} \qquad C_{-1}^{(2)} = \begin{pmatrix} & & \frac{\sqrt{2}\mathrm{i}}{2} \\ & \frac{i}{2} & \\ -\frac{\sqrt{3}}{2} & & \\ 0 & & \\ 0 & & 0 \end{pmatrix} \qquad C_{0}^{(2)} = \begin{pmatrix} 0 & & 0 \\ & & \frac{\sqrt{3}\mathrm{i}}{2} \\ & 0 & \\ -\frac{\sqrt{3}\mathrm{i}}{2} & & \\ 0 & & 0 \end{pmatrix}$$

$$C_{1}^{(2)} = \begin{pmatrix} 0 & & 0 \\ & & 0 \\ & & \frac{\sqrt{3}\mathrm{i}}{2} \\ & -\frac{\mathrm{i}}{2} & \\ -\frac{\sqrt{2}\mathrm{i}}{2} & & \end{pmatrix} \qquad C_{2}^{(2)} = \begin{pmatrix} 0 & & 0 \\ & & 0 \\ & & 0 \\ & & \frac{\sqrt{2}\mathrm{i}}{2} \\ 0 & -\mathrm{i} & \end{pmatrix}$$

$$C_{-3}^{(3)} = \begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & & \\ 0 & & \\ 0 & & \\ 0 & & 0 \end{pmatrix} \qquad C_{-2}^{(3)} = \begin{pmatrix} & \frac{1}{3} & 0 \\ \frac{\sqrt{2}}{3} & & \\ 0 & & \\ 0 & & \\ 0 & & 0 \end{pmatrix}$$

$$
C_{-1}^{(3)} = \begin{pmatrix} & & \frac{\sqrt{5}}{15} \\ & \frac{2\sqrt{10}}{15} & \\ \frac{\sqrt{30}}{15} & & \\ 0 & & \\ 0 & & 0 \end{pmatrix} \qquad
C_{0}^{(3)} = \begin{pmatrix} 0 & & 0 \\ & & \frac{\sqrt{15}}{15} \\ & \frac{\sqrt{5}}{5} & \\ \frac{\sqrt{15}}{15} & & \\ 0 & & 0 \end{pmatrix} \qquad
C_{1}^{(3)} = \begin{pmatrix} 0 & & 0 \\ & & 0 \\ & & \frac{\sqrt{30}}{15} \\ & \frac{2\sqrt{10}}{15} & \\ \frac{\sqrt{5}}{15} & & \end{pmatrix}
$$

$$
C_{2}^{(3)} = \begin{pmatrix} 0 & & 0 \\ & & 0 \\ & & 0 \\ & & \frac{\sqrt{2}}{3} \\ 0 & \frac{1}{3} & \end{pmatrix} \qquad
C_{3}^{(3)} = \begin{pmatrix} 0 & & 0 \\ & & 0 \\ & & 0 \\ & & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}
$$

where missing matrix entries are all zero. It is straightforward to verify that $\mathbf{C}^{5\times 3}$ is decomposed into the orthogonal direct sum

$$
\mathbf{C}^{5\times 3} = \mathrm{span}\{C_n^{(1)}\}_{|n|\leqslant 1} \oplus \mathrm{span}\{C_m^{(2)}\}_{|m|\leqslant 2} \oplus \mathrm{span}\{C_k^{(3)}\}_{|k|\leqslant 3} \tag{112}
$$

with respect to the inner product $\langle C_1, C_2\rangle = \mathrm{tr}(C_1^* C_2)$. This decomposition is a realization of

$$
\mathbf{C}^{5\times 3} \cong \mathbf{C}^5 \otimes \mathbf{C}^3 \cong V_1 \oplus V_2 \oplus V_3. \tag{113}
$$

The decomposition (112) gives rise to a realization of the decomposition (104) as

$$
H^2(\mathbf{R}^3_\xi) \otimes H^1(\mathbf{R}^3_\eta) \cong \mathrm{span}\{u_n^{(1)}(\boldsymbol{\xi}, \boldsymbol{\eta})\} \oplus \mathrm{span}\{u_m^{(2)}(\boldsymbol{\xi}, \boldsymbol{\eta})\} \oplus \mathrm{span}\{p_k^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta})\}. \tag{114}
$$

This shows that the polynomials $p_k^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ are basis polynomials of V_3. Furthermore, for $\boldsymbol{\xi} = \boldsymbol{\eta} = \boldsymbol{x}$, $p_k^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ reduce to spherical harmonics

$$
p_k^{(3)}(\boldsymbol{x}, \boldsymbol{x}) = \sqrt{\frac{8\pi}{105}} r^3 Y_{3k}(\theta, \phi) \qquad |k| \leqslant 3 \tag{115}
$$

which transform exactly according to

$$
p_k^{(3)}(g^{-1}\boldsymbol{x}, g^{-1}\boldsymbol{x}) = \sum_{|k'|\leqslant 3} p_{k'}^{(3)}(\boldsymbol{x}, \boldsymbol{x}) D^3_{k'k}(g). \tag{116}
$$

Since the representation of $SO(3)$ in V_3 is irreducible and unique up to equivalence, the polynomials $p_k^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta})$ should be subject to the transformation

$$
p_k^{(3)}(g^{-1}\boldsymbol{\xi}, g^{-1}\boldsymbol{\eta}) = \sum_{|k'|\leqslant 3} p_{k'}^{(3)}(\boldsymbol{\xi}, \boldsymbol{\eta}) D^3_{k'k}(g). \tag{117}
$$

Acknowledgment

This work was partly supported by the Grant-in-Aid for Scientific Research of the Ministry of Education, Culture, Sports, Science and Technology of Japan.

References

[1] Guichardet A 1984 On rotation and vibration motions of molecules *Ann. Inst. H. Poincaré Phys. Theor.* **40** 329–42

[2] Tachibana A and Iwai T 1986 Complete molecular Hamiltonian based on the Born-Oppenheimer adiabatic approximation *Phys. Rev.* A **33** 2262–9

[3] Iwai T 1987 A gauge theory for the quantum planar three-body problem *J. Math. Phys.* **28** 964–74

[4] Iwai T 1987 A geometric setting for internal motions of the quantum three-body system *J. Math. Phys.* **28** 1315–26

[5] Iwai T 1988 A geometric setting for the quantum planar n-body system, and a $U(n-1)$ basis for the internal states *J. Math. Phys.* **29** 1325–37

[6] Iwai T 1999 Classical and quantum mechanics of jointed rigid bodies with vanishing total angular momentum *J. Math. Phys.* **40** 2381–99

[7] Littlejohn R G and Reinsch M 1997 Gauge fields in the separation of rotations and internal motions in the n-body problem *Rev. Mod. Phys.* **69** 213–75

[8] Tanimura S and Iwai T 2000 Reduction of quantum systems on Riemannian manifolds with symmetry and application to molecular mechanics *J. Math. Phys.* **41** 1814–42

[9] Mitchell K A and Littlejohn R G 2000 Boundary conditions on internal three-body wavefunctions *Phys. Rev.* A **61** 042502-1–042502-16

[10] Littlejohn R G, Mitchell K A and Reinsch M 1998 Internal spaces, kinetic rotations and body frames for four-atom sytem *Phys. Rev.* A **58** 3718–38

[11] Mitchell K A and Littlejohn R G 2002 Kinematic orbits and the structure of the internal space for systems of five or more bodies *J. Phys. A: Math. Gen.* **33** 1395–1416

[12] Rose M E 1957 *Elementary Theory of Angular Momentum* (New York: Wiley)

[13] Iwai T and Yamaoka H 2003 Stratified reductuion of many-body kinetic energy operators *J. Math. Phys.* **44** 4411–35

[14] Weyl H 1950 *The Theory of Groups and Quantum Mechanics* (New York: Dover)

[15] Iwai T and Hirose T 2002 The reduction of a quantum system of three identical particles on a plane *J. Math. Phys.* **43** 2907–26

[16] Raynal J and Revai J 1970 Transformation coefficients in the hyperspherical approach to the three-body problem *Nuovo Cimento* A **68** 612–22