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Boundary conditions at singular configurations of three-body systems

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Abstract

For some time, singular configurations have not been taken into account in dealing with the center-of-mass system of many particles. This is because the center-of-mass system can be made into a fiber bundle, provided the configurations of particles are restricted to non-singular ones. This article is an attempt to analyzing the center-of-mass system with configurations including the singular ones, and we present the condition for which a wave function must satisfy, should the particle configuration become singular in finite time. This article should give a similar result to [2], but from a completely different view point.

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1 Introduction

It is well known that reducing a dynamical system is closely related to a symmetry. One famous example is the reduction of quantum system. One may consider an eigenvalue problem for angular momentum, and would find that the eigenstate is a product of the radial and spherical harmonic functions. Then the original Schrödinger's equation is reduced to the one for finding the unknown radial function. That way, the system's degrees of freedom is reduced to a lower value.

The above mentioned reduction is a fine example of the heart of this subject. The two-body angular momentum problem happens to be a particular example of the Fourier analysis on $SO(3)$ for the three-body one.

1.1 Historical background

The idea of viewing many-particle center-of-mass system as a principal fiber bundle is in fact fairly new. However, there had been many painful attempts to separate rotation from vibrations. It was Guichardet, in 1984 who first defined rotational and vibarational vectors, and showed that the rotation can not be separated from vibrations, using the connection theory, provided that the particles do not collide nor align in a straight line. As a consequence, it was shown that any rotation angle of the particles were possible, purely by vibrations. In 1987, one of the authors (T.I) showed that if the system is restricted to regular configurations, it can be described in the bundle picture, in the sense that the behavior of the system can be discussed on associate vector bundle of the configuration space. Further, in 1990 and 1991, Montgomery defined the falling cat problem, and showed the cat constructed from point particles, can land on her feet when she is launched in air. This was done by viewing the system from a bundle picture with non-holonomic constraints. However, one must realize that all above articles dealt with center-of-mass systems with the free action of $SO(3)$. The consequence of this automatically excludes the cases when particles collide at the origin, or are aligned in a line. These mentioned cases are called the singular configurations, and the questions on how the mechanics is set up on such configurations are still unsolved. This article deals with such a question.

1.2 Organization of the article

This article is organized as follows. After this chapter, in section 2 we give a brief review of the center-of-mass system. The definition of regular and singular configurations is given in this chapter, and gives a brief idea as to what can be done with regular configurations. The most of the facts mentioned in the chapter are already investigated and cooked by past researchers. For a beginner to this subject, we suggest it would be of great help to start from reading [3]. One may wonder whether it would be possible for a system to come to a singular configuration from a regular one in finite time. Demonstration of this is given in section 3. It further gives us a motivation to see the behavior of a quantum system instead of classical ones. Also a wavefunction can be written in a tidy form by introducing something called the *projection* and *transition operators*. These operators have remarkable properties, and they are described in this section, too. In section 4, we work through two examples. The main theme in this section is to write wavefunction in terms of local coordinates, given that it is analytic and that can be expanded into power series around a singular configuration. One of the main results of the article is also describen in this section. Section 5 deals with the expansion of the wavefunction when triple collision takes place, stating the other main result.

2 Review of the center-of-mass system

As is widely discussed, the center-of-mass system has been very well studied by past mathematicians and physicists. In this section we shall concentrate on some of the well known facts.

2.1 Set–up of the problem

Out of n particles, let $\boldsymbol{x}_j \in \mathbb{R}^3$ be the position of jth particle, and m_j be its respective mass. Then we define the configuration space of the center–of–mass system to be

$$X_0 = \left\{ x = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_n) \mid \boldsymbol{x}_j \in \mathbb{R}^3, \sum_{j=1}^{n} m_j \boldsymbol{x}_j = 0 \right\}. \tag{1}$$

The translational motion of particles are deliberately removed, and the consequence of this appears in the constraint

$$\sum_{j=1}^{j=n} m_j \boldsymbol{x}_j = 0 \tag{2}$$

in X_0, in order to fix the center of mass at the origin. This configuration space allows a group action of $SO(3)$, and this is given by

$$SO(3) \times X_0 \longrightarrow X_0, \qquad (g, x) \mapsto gx = (g\boldsymbol{x}_1, \dots, g\boldsymbol{x}_n). \tag{3}$$

2.2 A variety of configurations

When n particles are placed in $\mathbb{R}^3$, we may consider how the particles are arranged in that space. Therefore, we define the spread of particles to be

$$F_x = \operatorname{span}\{\boldsymbol{x}_1, \dots, \boldsymbol{x}_n\}, \qquad x \in X_0. \tag{4}$$

Then

$$\dim F_x = 0 \ : \ \text{all particles at the origin} \tag{5}$$
$$\dim F_x = 1 \ : \ \text{particles aligned in a line} \tag{6}$$
$$\dim F_x = 2 \ : \ \text{particles on a plane} \tag{7}$$
$$\dim F_x = 3 \ : \ \text{particles scattered in space.} \tag{8}$$

From this, we see that there are different configurations for different dimensions of F_x.

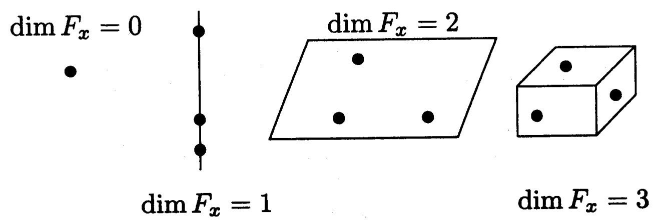

Figure 1: The diagram shows the interpretations of the dimensions of F_x. From left, corresponds to 1) all particles at the origin, 2) particles aligned in a line, 3) particles on a plane, 4) particles scattered in space.

This suggests us to break the configuration space X_0 up into subspaces Q_0, Q_1, and $\dot{Q}$;

$$\begin{aligned} Q_0 &= \{x \in X_0 \mid \dim F_x = 0\} = \{0\} & (9) \\ Q_1 &= \{x \in X_0 \mid \dim F_x = 1\} & (10) \\ \dot{Q} &= \{x \in X_0 \mid \dim F_x \geq 2\}. & (11) \end{aligned}$$

The members of Q_0 and Q_1 are the configurations for colliding particles and aligned particles respectively, and such configurations are called the *singular configurations.*

2.3 Restriction to regular configurations

For a fixed $x \in X_0$, an isotropy subgroup G_x of $SO(3)$ is the subgroup of $SO(3)$ which makes x invariant under the action of $g \in G_x$. For different members of X_0, we have different isotropy subgroups;

$$G_x \cong \begin{cases} SO(3) & (x \in Q_0) \\ SO(2) & (x \in Q_1) \\ \{e\} & (x \in \dot{Q}). \end{cases} \tag{12}$$

For $x \in \dot{Q}$, $G_x \cong \{e\}$, so action $SO(3)$ is free. Therefore $\dot{Q} = \{x \in X \mid \dim F_x \geq 2\}$ is made in to an $SO(3)$ bundle through the equivalence relation $\sim$

$$y \sim x \iff \exists g \in SO(3) \quad s.t. \quad y = gx \tag{13}$$

for $x, y \in \dot{X}$, with the quotient map

$$\pi : \dot{Q} \longrightarrow M := \dot{Q}/SO(3) = \{[x] \mid x \in X_0\}. \tag{14}$$

Then we shall define open set U in M by the following statement. A subset U of M is an open subset of M for the quotient topology if and only if its inverse image

$$\pi^{-1}(U) = \{x \in X_0 \mid [x] \in U\} \tag{15}$$

is an open subset of X_0. For a given $U \subset M$, its inverse image has a local structure $\pi^{-1}(U) \cong U \times G$. We define *section* σ in $\pi^{-1}(U)$ to be the continuous map

$$\sigma : M \supset U \longrightarrow X_0. \tag{16}$$

Then further, we have an associated bundles

$$E_l = \dot{Q} \times_l \mathcal{H}^l := \dot{Q} \times \mathcal{H}^l / \sim \tag{17}$$

defined through

$$(x, z) \sim (gx, \mathcal{D}^l(g)z) \in \dot{Q} \times \mathcal{H}^l \tag{18}$$

where $\mathcal{H}^l$ is the representation space of $SO(3)$ with

$$\dim \mathcal{H}^l = 2l + 1. \tag{19}$$

Like before, one can define section of the associated vector bundle

$$\sigma_l : \dot{Q}/SO(3) \longrightarrow \dot{Q} \times_l \mathcal{H}^l, \tag{20}$$

being interpreted as a reduced state, because the reduced state is in one to one correspondence with σ_l.

3 Taking singular configurations into account

The previous argument of vector bundles in section 2 was all good provided that the action of $SO(3)$ was free. However this is not the case for the singular configurations. Such configurations have $G_x \not\cong \{e\}$. In this section we shall consider configurations including the singular ones.

Before we start, one might be led to a natural question whether or not it would be possible for a natural dynamical system to come to a singular configuration in finite time. To answer the question, we shall manulally construct a colinear configuration for the free particles.

3.1 Construction of colliding free particles

For simplicity, we shall only consider three free particles in space, that is, for each $\boldsymbol{x}_j$, $j = 1, 2, 3$, $\boldsymbol{x}_j \in \mathbb{R}^3$, $\boldsymbol{x}_j$ is linear in time t. Since the configuration space can be identified with set of Jacobi vectors, from now on we shall work in terms of Jacobi vectors. The Jacobi vectors are given by the following formulae

$$\boldsymbol{r}_1 = \sqrt{\frac{m_1 m_2}{m_1 + m_2}} (\boldsymbol{x}_2 - \boldsymbol{x}_1) \tag{21}$$

$$\boldsymbol{r}_2 = \sqrt{\frac{m_1 m_2 (m_1 + m_2)}{m_1 + m_2 + m_3}} \left(\boldsymbol{x}_3 - \frac{m_1 \boldsymbol{x}_1 + m_2 \boldsymbol{x}_2}{m_1 + m_2} \right) \tag{22}$$

for $\boldsymbol{r}_j \in \mathbb{R}^3$. Jacobi vectors are just a linear combination of $\boldsymbol{x}_j$'s, so we see that they are also linear with respect to t. This gives the form of Jacobi vectors;

$$\boldsymbol{r}_1 = \boldsymbol{a}_1 + \boldsymbol{b}_1 t \tag{23}$$

$$\boldsymbol{r}_2 = \boldsymbol{a}_2 + \boldsymbol{b}_2 t \tag{24}$$

for constant vectors $\boldsymbol{a}_j, \boldsymbol{b}_j \in \mathbb{R}^3$, and $t \in \mathbb{R}$. Here assume that neither $\boldsymbol{r}_1$ nor $\boldsymbol{r}_2$ vanishes. Then when particles form a colinear shape, we have

$$\boldsymbol{r}_1 \times \boldsymbol{r}_2 = 0 \qquad \text{for some } t_c \in \mathbb{R} \tag{25}$$

or equivalently

$$\boldsymbol{r}_1 = \lambda \boldsymbol{r}_2 \qquad \text{for some } t_c, \lambda \in \mathbb{R}. \tag{26}$$

Here we can consider two cases. Case one is when $\boldsymbol{r}_1 \times \boldsymbol{r}_2 = 0$ and case two when $\boldsymbol{r}_2 \times \boldsymbol{r}_2 \neq 0$. If it is the former case, then it is trivial to see that if the plane spanned by $\boldsymbol{a}_1$, O, $\boldsymbol{r}_1(t)$ and that by $\boldsymbol{a}_2$, O, $\boldsymbol{r}_2(t)$ do not coincide, then we do have a colinear configuration. Therefore we shall consider the latter case, that is, $\boldsymbol{r}_1 \times \boldsymbol{r}_2 \neq 0$. Here we note that if there is a colinear shape, then the loci of $\boldsymbol{r}_1$ is in the plane spanned by $\boldsymbol{a}_1$, O, $\boldsymbol{r}_1(t_c)$. We shall call this plane P_1. Similarly, the loci of $\boldsymbol{r}_1$ should be in the plane spanned by $\boldsymbol{a}_2$, O, $\boldsymbol{r}_2(t_c)$. Again we shall call this plane P_2.

We are now in position to construct a colinear configuration manually. In this example, we let P_1 and P_2 coincide. Choose $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ so that they satisfy $\boldsymbol{a}_1 \cdot \boldsymbol{b}_1 = 0$,

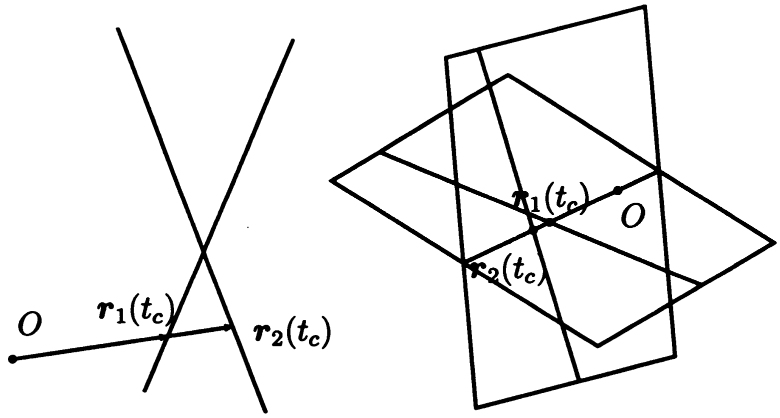

Figure 2: The lines show the loci of two Jacobi vectors with respect to time. The diagram on the left describes how two skewing loci can come to a configuration which gives parallel Jacobi vectors. Similarly the diagram on the right shows it in the three dimensional manner. Planes drawn are P_1 and P_2. This shows that the intersection of the planes must be in the direction of parallel Jacobi vectors.

and $\boldsymbol{a}_2 \cdot \boldsymbol{b}_2 = 0$. This means that we may assume that $\boldsymbol{a}_j$ and $\boldsymbol{b}_j$ are perpendicular, without loss of generality. For given $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, the plane defined by $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, O is

$$\boldsymbol{r} = \alpha_1 \boldsymbol{a}_1 + \alpha_2 \boldsymbol{a}_2 \qquad \alpha_1, \alpha_2 \in \mathbb{R}. \tag{27}$$

So for chosen $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, we then choose $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ such that the loci $\boldsymbol{r}_1(t)$, and $\boldsymbol{r}_2(t)$ lie on the plane(s)

$$\hat{\boldsymbol{b}}_1 \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2) = 0 \qquad \hat{\boldsymbol{b}}_2 \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2) = 0 \tag{28}$$

If we set $\lambda = 1$, then at the linear configuration, we must have $\boldsymbol{r}_1(t_c) = \boldsymbol{r}_2(t_c)$, where t_c is the time at which colinear configuration takes place. Now note that we may change the time scales of loci of Jacobi vecotors in the following way

$$\boldsymbol{r}_1 = \boldsymbol{a}_1 + |\boldsymbol{b}_1|\hat{\boldsymbol{b}}_1 t = \boldsymbol{a}_1 + \hat{\boldsymbol{b}}_1 t_1 \tag{29}$$

$$\boldsymbol{r}_2 = \boldsymbol{a}_2 + |\boldsymbol{b}_2|\hat{\boldsymbol{b}}_2 t = \boldsymbol{a}_2 + \hat{\boldsymbol{b}}_2 t_2 \tag{30}$$

Then, now we solve for the time at which these loci intersect. If t^* is such time, then

$$\boldsymbol{a}_1 + \hat{\boldsymbol{b}}_1 t_1^* = \boldsymbol{a}_2 + \hat{\boldsymbol{b}}_2 t_2^*. \tag{31}$$

Now, if we set t^* such that it satisfies

$$\frac{|\hat{\boldsymbol{b}}_1 t_1|}{|\hat{\boldsymbol{b}}_2 t_2|} = \frac{\text{speed of } \boldsymbol{r}_1}{\text{speed of } \boldsymbol{r}_2} = \frac{t_1^*}{t_2^*} = \frac{|b_1|}{|b_2|}, \tag{32}$$

then we have particles aligned in straight line. If we further set $\boldsymbol{b}_1$ to be a unit vector, then the Jacobi vectors in this case are

$$\boldsymbol{r}_1 = \boldsymbol{a}_1 + \hat{\boldsymbol{b}}_1 t \tag{33}$$

$$\boldsymbol{r}_2 = \boldsymbol{a}_2 + \frac{t_2^*}{t_1^*}\hat{\boldsymbol{b}}_2 t. \tag{34}$$

The configurations corresponding to Jacobi vectors (33–34) are regular except for when $t = t_1^*$.

3.2 The total angular momentum of singular configuration

For free particles, the total angular momentum of the system is given by

$$L = \sum_{j=1}^{2} \boldsymbol{r}_j \times \frac{d\boldsymbol{r}_j}{dt} \tag{35}$$

$$= (\boldsymbol{a}_1 + \boldsymbol{b}_1 t) \times \boldsymbol{b}_1 + (\boldsymbol{a}_2 + \boldsymbol{b}_2 t) \times \boldsymbol{b}_2 \tag{36}$$

$$= \boldsymbol{a}_1 \times \boldsymbol{b}_1 + \boldsymbol{a}_2 \times \boldsymbol{b}_2 \tag{37}$$

$$= \text{constant}. \tag{38}$$

When singular configuraion undergoes, the directions of $\boldsymbol{r}_1(t_c)$ and $\boldsymbol{r}_2(t_c)$ coincide. Then the angular momentum about the colinear axis is

$$\boldsymbol{n} \cdot L = \boldsymbol{n} \cdot (\boldsymbol{a}_1 \times \boldsymbol{b}_1 + \boldsymbol{a}_2 \times \boldsymbol{b}_2) \tag{39}$$

$$= \boldsymbol{n} \cdot (\boldsymbol{a}_1 \times \boldsymbol{b}_1) + \boldsymbol{n} \cdot (\boldsymbol{a}_2 \times \boldsymbol{b}_2) \tag{40}$$

$$= \boldsymbol{r}_1(t_c) \cdot (\boldsymbol{a}_1 \times \boldsymbol{b}_1) + \lambda \boldsymbol{r}_2(t_c) \cdot (\boldsymbol{a}_2 + \boldsymbol{b}_2) \tag{41}$$

$$= 0, \tag{42}$$

where

$$\boldsymbol{n} = \boldsymbol{r}_1(t_c). \tag{43}$$

This indicates that any free particles, at its singular configuration would have a zero angular momentum about its axis. It then makes us wonder if this result would be the same for the quantum center-of-mass system.

These particles under no external force may travel in straight lines in X_0. The corresponding motions in $X_0/SO(3)$ can be represented in local coordinates (η_1, η_2, η_3), where

$$\eta_1 = \boldsymbol{r}_1^2 - \boldsymbol{r}_2^2 = (\boldsymbol{a}_1^2 - \boldsymbol{a}_2^2) + (\boldsymbol{b}_1^2 - \boldsymbol{b}_2^2)t^2 \tag{44}$$

$$\eta_2 = 2\boldsymbol{r}_1 \cdot \boldsymbol{r}_2 = 2(\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 + \boldsymbol{b}_1 \cdot \boldsymbol{b}_2 t^2) \tag{45}$$

$$\eta_3 = 2|\boldsymbol{r}_1 \times \boldsymbol{r}_2| = 2[\boldsymbol{a}_1 \times \boldsymbol{a}_2 + \boldsymbol{b}_1 t \times \boldsymbol{a}_2 + \boldsymbol{a}_1 \times \boldsymbol{b}_2 t + \boldsymbol{b}_1 \times \boldsymbol{b}_2 t^2]. \tag{46}$$

The singular configuration, as one can see, corresponds to the plane $\eta_3 = 0$.

3.3 Fourier Analysis

From what we know, we have the group action

$$SO(3) \times X_0 \longrightarrow X_0 \tag{47}$$

We shall consider a quantum system with wave functions in $L^2(X_0)$, and unitary representation $U : SO(3) \times L^2(X_0) \longrightarrow L^2(X_0)$, defined by

$$(g, f) \mapsto U(g)f; \qquad (U(g)f)(x) = f(g^{-1}x). \tag{48}$$

As what the unitary representation show, f is defined on the configuration space X_0. However, suppose that $x \in X_0$ is fixed, and let us define

$$f_x(g) := f(gx), \tag{49}$$

then we can see that f_x is a function on $SO(3)$. Later if we require it to be that of X_0, then we can simply put $g = e$, and we revert to the function f evaluated at the point $x \in X_0$.

Now, since f can be seen as a function on $SO(3)$, we can apply the Peter–Weyl theorem, which allows us to expand functions on compact Lie groups. Then the Fourier expansion of f is expressed as

$$f(gx) = \sum_{l=0}^{\infty}(2l+1) \sum_{|m|,|n|\leq l} \mathcal{D}^l_{mn}(g)\langle \mathcal{D}^l_{mn}, f_x\rangle_{SO(3)}, \tag{50}$$

where $\langle\ ,\ \rangle_{SO(3)}$ denotes the inner product for functions on $SO(3)$

$$\langle \mathcal{D}^l_{mn}, f_x\rangle_{SO(3)} = \int_{SO(3)} \overline{\mathcal{D}}^l_{mn}(k) f(kx) d\mu(k). \tag{51}$$

Above expansion holds for all $g \in SO(3)$, so for $g = e$ in particular, we have

$$f(x) = \sum_{l=0}^{\infty}(2l+1)\sum_{|m|\le l}\int_{SO(3)} \overline{\mathcal{D}}^l_{mm}(h) f(hx) d\mu(h). \tag{52}$$

The $d\mu(h)$ is the invariant measure for $SO(3)$. When it is expressed in tems of the local coordinates, we have

$$d\mu(h) = \sin\theta d\theta d\phi d\psi / 2\pi^2 \qquad \text{with} \qquad \int_{SO(3)} d\mu(h) = 1, \tag{53}$$

where (θ, ϕ, ψ) are the *Euler angles.*

3.4 Projection and Transition Operators

Here, in order to write equation (52) in a neater manner, we introduce operators P^l

$$(P^l_n f)(x) = (2l+1)\int_{SO(3)} \mathcal{D}^l_{nn}(h) f(h^{-1}x) d\mu(h) \tag{54}$$

$$(P^l_{mn} f)(x) = (2l+1)\int_{SO(3)} \mathcal{D}^l_{mn}(h) f(h^{-1}x) d\mu(h). \tag{55}$$

Equations (54–55) have the following properties;

$$(P^l_n)^\dagger = P^l_n, \qquad P^l_n P^l_m = \delta_{nm} P^l_n \tag{56}$$

$$P^l_{nm}(P^l_{nm})^\dagger = P^l_n, \quad P^l_{nm}P^l_m = P^l_n P^l_{nm}, \quad P^l_{nm} : \mathrm{Im}P^l_m \longrightarrow \mathrm{Im}P^l_n \tag{57}$$

The most striking properties are the last equations from (56) and (57). Equation (56) says that applying P^l_n twice has the same effect as applying it only once, whereas equation (57) says the map P^l_{nm} shifts a point in $\mathrm{Im}P^l_m$ to that of n. For the above reasons, we shall from here call the operators in (54) and (55) *projection* and *transition operators* respectively. Further, these operators can be written in a slightly different manner since

$$\int_{SO(3)} \mathcal{D}^l_{mn}(h) f(h^{-1}x) d\mu(h) = \int_{SO(3)} \overline{\mathcal{D}}^l_{nm}(k) f(kx) d\mu(k). \tag{58}$$

by change of variables $h = k^{-1}$. Then we have

$$(P^l_{mn}f)(x) = (2l+1)\int_{SO(3)} \overline{\mathcal{D}}^l_{nm}(k)f(kx)d\mu(k) \tag{59}$$

So Fourier series expansions (52) in x is;

$$f(x) = \sum_{l=0}^{\infty}\sum_{|m|\le l}(P^l_m f)(x). \tag{60}$$

Now define map $E^l_m : L^2(X_0) \longrightarrow \mathcal{H}^l \otimes L^2(X_0)$;

$$E^l_m f = \frac{1}{\sqrt{2l+1}}\begin{pmatrix} P^l_{lm}f \\ P^l_{l-1m}f \\ \vdots \\ P^l_{-lm}f \end{pmatrix} \tag{61}$$

Satisfies the condition

$$(E^l_m f)(hx) = \mathcal{D}^l(h)(E^l_m f)(x), \qquad h \in SO(3). \tag{62}$$

This means that the $\mathcal{H}^l$-valued functions $E^l_m f$ are ρ^l-equivariant functions. Here we did not specify nor say anything about form of f or the point x, and therefore this condition is true for any configuration including the singular ones.

4 Wavefunctions around singular configurations

In this section of the article, we shall try to write (60) and hence (52) in terms of local sections of X_0. However, for the simplicity, we shall consider 3-body system.

We have already seen that the space of center-of-mass system is identified with the space of coulpled Jacobi vectors (21–22) in terms of vector spaces

$$X_0 \cong \left\{(\boldsymbol{r}_1, \boldsymbol{r}_2) \mid \boldsymbol{r}_j \in \mathbb{R}^3, j = 1, 2\right\}. \tag{63}$$

At singular configuration, $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ become parallel to each other, and they are linearly dependent. Further, we define

$$M := X_0/SO(3) \cong \{\boldsymbol{x} \in \mathbb{R}^3 \mid x_3 \ge 0\}. \tag{64}$$

the internal space of the whole of X_0. The whole of X_0 includes the singular configurations. As already stated, M fails to be a manifold. However, we see that

$$\pi(\partial\dot{X}) = \partial\pi(\dot{X}), \tag{65}$$

and so the boundary gets mapped to the boundary. We say that M is a *manifold with boundary.*

Away from the boundary, there are three coordinate variables, and we define them to be $(r_1, r_2, \varphi) \in M$ such that

$$r_1 = |\boldsymbol{r}_1|, \quad r_2 = |\boldsymbol{r}_2|, \quad \boldsymbol{r}_1 \cdot \boldsymbol{r}_2 = r_1 r_2 \cos\varphi. \tag{66}$$

The boundary of M is identified with $\varphi = 0$. Further, choose local section $\sigma : U \subset M \longrightarrow X_0$:

$$(r_1, r_2, \varphi) \mapsto \zeta = (r_1 e_3, r_2 e^{\varphi R(e_2)} e_3), \quad R : \mathbb{R}^3 \longrightarrow so(3), \tag{67}$$

then any point in $\pi^{-1}(U)$ is expressed as $x = g\zeta$, and expansion of f takes the form:

$$f(g\zeta) = \sum_{l=0}^{\infty}(2l+1) \sum_{|m|,|n|\le l} \mathcal{D}^l_{mn}(g)\langle \mathcal{D}^l_{mn}, f_\zeta\rangle_{SO(3)} \tag{68}$$

where $f_\zeta(k) = f(k\zeta)$ for $k \in SO(3)$. Further, this in terms of P^l_{nm} is

$$f(g\zeta) = \sum_{l=0}^{\infty} \sum_{|m|,|n|\le l} \mathcal{D}^l_{mn}(g)(P^l_{nm} f)(\zeta) \tag{69}$$

The equivariance condition (62) which is equivalent for the ζ expansion is

$$(E^l_m f)(g\zeta) = \mathcal{D}^l(g)(E^l_m f)(\zeta). \tag{70}$$

4.1 Two worked examples

It comes very natural for us to investigate the behavior of wavefunctions at the singular and near–singular configurations. Here we shall choose sections to represent these configurations. Of the two examples, first, we shall look into the case when we have a colinear singular configuration.

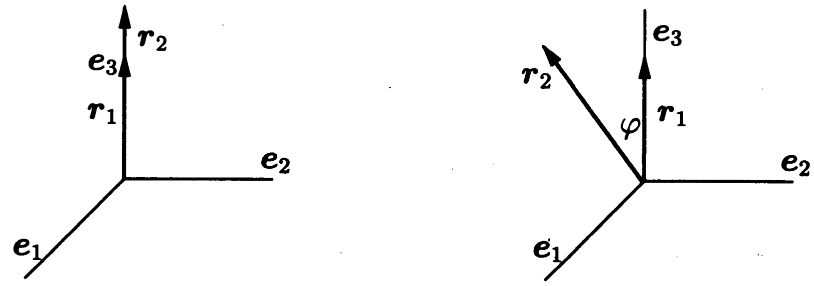

Figure 3: Section for the colinear singular configuration (left) and that for the near–singular configuration (right). Notice the decrease in dimension in the singular configuration.

The boundary of M can be represented by local coordinates (r_1, r_2), and we shall consider the following section

$$\partial M \ni (r_1, r_2) \mapsto \zeta_0 = (r_1 e_3, r_2 e_3) \in X_0 \tag{71}$$

and here we note that the isotropy subgroup of $SO(3)$ at ζ_0 and it's representation are

$$g = e^{tR(e_3)}, \quad \mathcal{D}^l_{nm}(g) = e^{-itn}\delta_{nm}, \quad t \in \mathbb{R} \tag{72}$$

respectively. Now, as already mentioned, the equivariance condition (70) holds for any $g \in SO(3)$. So in particular, for $g \in G_{\zeta_0}$, the action of P^l_{nm} on f is

$$\begin{aligned} (P^l_{nm}f)(\zeta_0) &= (P^l_{nm}f)(g\zeta_0) && (73)\\ &= \sum_{|n'|\le l} \mathcal{D}^l_{nn'}(g)(P^l_{n'm}f)(\zeta_0) && (74)\\ &= \sum_{|n'|\le l} e^{-int}\delta_{nn'}(P_{n'm}f)(\zeta_0) && (75)\\ &= e^{-int}(P^l_{nm}f)(\zeta_0). && (76) \end{aligned}$$

We used two facts here. One is that ζ_0 is invariant under $g \in G_{\zeta_0}$. The other is the equivariance. Furthermore the bove equations (73–76) is just the calculation of (70) component wise, since the matrix $\mathcal{D}^l$ is diagonal in this case. The consequence of the condition is that

$$(P^l_{nm}f)(\zeta_0) = 0 \quad \text{if} \quad n \neq 0. \tag{77}$$

We have the physical interpretation on the result (77) as follows: For a colinear configuration with a given angular momentum n around the axis of alignment, the wave function must vanish for this configuration, unless the angular momentum is zero. In other words, we have no probablity of finding colinear configuration if there is a non zero angular momentum round that axis.

Using this result, we may further calculate (52) by letting ζ tend to ζ_0. Then we obtain

$$f(g\zeta_0) = \sum_{l=0}^{\infty}\sum_{|m|,|n|\leq l} \mathcal{D}^l_{mn}(g)(P^l_{nm}f)(\zeta_0) \tag{78}$$

$$= \sum_{l=0}^{\infty}\sum_{|m|\leq l} \mathcal{D}^l_{m0}(g)(P^l_{0m}f)(\zeta_0) \tag{79}$$

$$= \sum_{l=0}^{\infty}\sum_{|m|\leq l} \sqrt{\frac{4\pi}{2l+1}}\overline{Y}_{lm}(ge_3)(P^l_{0m}f)(\zeta_0). \tag{80}$$

This implies that the wave functions for linear triatomic molecues can be described in terms of local coordinates, (θ, ϕ, r_1, r_2), in the subspace of X_0 determined by rank $(\boldsymbol{r}_1, \boldsymbol{r}_2) = 1$. As a side note, recall that two-body system can be characterized by considering the section

$$r \mapsto \zeta_0 = r\boldsymbol{e}_3 \tag{81}$$

Then Fourier expansion is

$$f(g\zeta_0) = \sum_{l=0}^{\infty}\sum_{|m|\leq l} \sqrt{\frac{4\pi}{2l+1}}\overline{Y}_{lm}(ge_3)(P^l_{0m}f)(\zeta_0). \tag{82}$$

Actually $(P^l_{0m}f)(\zeta_0)$ is dependent only on r. The system is then reduced to wavefunction for the radial component.

4.2 Three particles in the nbd of a linear configuration

As before, we shall choose a section for configurations very close to the singular one. For point p which lies in the interior of M, we may write p in coordinates (r_1, r_2, φ). Then we may choose the section to be

$$(r_1, r_2, \varphi) \mapsto \zeta = (r_1\boldsymbol{e}_3, r_2 e^{\varphi R(e_2)}\boldsymbol{e}_3) \in X_0. \tag{83}$$

Because we are trying to express in terms of the local coordinates, we shall write out explicitly $k \in SO(3)$ in Euler angles

$$k = e^{\phi' R(e_3)} e^{\theta' R(e_2)} e^{\psi' R(e_3)} := k_0 e^{\psi' R(e_3)}. \tag{84}$$

Here we split $k \in SO(3)$ into two parts—namely k_0 and $e^{\psi' R(e_3)}$, because we are considering an expansion about the $\mathbf{e}_3$ axis. Then as before, we may write $x \in \pi^{-1}(U)$ as

$$x = k\zeta = k_0(r_1 \mathbf{e}_3, r_2 e^{\psi' R(e_3)} e^{\varphi R(e_2)} \mathbf{e}_3), \tag{85}$$

and recall that

$$\mathcal{D}^l_{mn}(k) = e^{-im\phi'} d^l_{mn}(\theta') e^{-in\psi'} \tag{86}$$

and we shall attempt to write (60) using those introduced variables. First we shall look into the calculation of $P^l_{nm} f$ that appears in (60).

$$\begin{aligned} (P^l_{nm} f)(\zeta) &= (2l+1) \int_{SO(3)} \overline{\mathcal{D}}^l_{mn}(k) f(k\zeta) d\mu(k) \\ &= (2l+1) \frac{1}{\pi} \int_{S^2} e^{im\phi'} d^l_{mn}(\theta') \sin\theta' d\theta' d\phi' \\ &\times \frac{1}{2\pi} \int_0^{2\pi} e^{in\psi'} f(r_1 k_0 \mathbf{e}_3, r_2 k_0 e^{\psi' R(e_3)} e^{\varphi R(e_2)} \mathbf{e}_3) d\psi' \end{aligned} \tag{87}$$

Observe that the last integral in (87) is a Fourier coefficient of $U(k_0^{-1}) f$;

$$\begin{aligned} &c_{-n}(k_0; r_1 \mathbf{e}_3, r_2 e^{\varphi R(e_2)} \mathbf{e}_3) \\ &= \frac{1}{2\pi} \int_0^{2\pi} e^{in\psi'} (U(k_0^{-1}) f)(r_1 \mathbf{e}_3, r_2 e^{\psi' R(e_3)} e^{\varphi R(e_2)} \mathbf{e}_3) d\psi'. \end{aligned} \tag{88}$$

Then (87) comes down to

$$(P^l_{nm} f)(\zeta) = (2l+1) \int_{SO(3)} \overline{\mathcal{D}}^l_{mn}(k) f(k\zeta) d\mu(k) \tag{89}$$

$$= \frac{1}{\pi} \int_{S^2} e^{im\phi'} d^l_{mn}(\theta') c_{-n}(k_0; r_1 \mathbf{e}_3, r_2 e^{\varphi R(e_2)} \mathbf{e}_3) \sin\theta' d\theta' d\phi' \tag{90}$$

We would like to take a closer look at these Fourier coefficients. To do so, we take a different set of Local coordinates $(r_1, r_2, \psi', \varphi) \mapsto (r_1, \xi_1, \xi_2, \xi_3)$, by setting

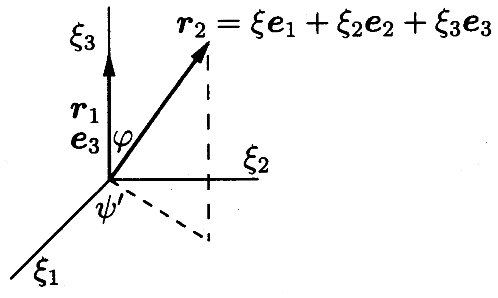

Figure 4: Changing the local coordinates. r_2, ϕ, ψ' are changed into cartesian coordinates in the standard way. Further change of variable gives z as viewing ξ_1–ξ_2 as the complex plane, and ρ as the modulus of $\boldsymbol{r}_2$ on the plane.

$$\xi_1 = r_2 \sin\varphi \cos\psi', \qquad \xi_2 = r_2 \sin\varphi \sin\psi', \qquad \xi_3 = r_2 \cos\varphi, \tag{91}$$

and we further put

$$z = \rho e^{i\psi'}, \qquad \rho = r_2 \sin\varphi. \tag{92}$$

The geographical interpretation for the lately introduced variables in (92) is that ρ is the length of r_2 when projected onto ξ_1–ξ_2 plane, and z is the complex variable when the plane spanned by (ξ_1, ξ_2) is identified as $\mathbb{C}$.

Now, assume the wave function is analytic in ξ_1 and ξ_2 at colinear singular configuration $\xi_1 = \xi_2 = 0$. We may expand $U(k_0^{-1})f$ into power series in the following way

$$\begin{aligned} &(U(k_0^{-1})f)(r_1\boldsymbol{e}_3, r_2 e^{\psi' R(\boldsymbol{e}_3)} e^{\varphi R(\boldsymbol{e}_2)} \boldsymbol{e}_3) \\ &= \sum_{p,q\geq 0}^{\infty} c_{pq}(k_0; r_1, \xi_3) z^p \bar{z}^q & (93) \\ &= \sum_{p,q\geq 0}^{\infty} c_{pq}(k_0; r_1, \xi_3) \rho^{p+q} e^{i(p-q)\psi'} & (94) \\ &= \sum_{n'=-\infty}^{\infty} e^{in'\psi'} \sum_{j=|n'|}^{\infty} \rho^j c_{\frac{j+n'}{2}, \frac{j-n'}{2}}(k_0; r_1, \xi_3), & (95) \end{aligned}$$

where c_{pq} are the coefficients of the power series. This implies that

$$c_{n'}(k_0; r_1\boldsymbol{e}_3, r_2 e^{\varphi R(\boldsymbol{e}_2)} \boldsymbol{e}_3) = \sum_{j=|n'|}^{\infty} \rho^j c_{\frac{j+n'}{2}, \frac{j-n'}{2}}(k_0; r_1, \xi_3) \tag{96}$$

with $n' = -n$. So $(P^l_{nm}f)(\zeta)$ turns out to be a power series of ρ having terms of the lowest order $|n|$;

$$
\begin{aligned}
(P^l_{nm}f)(\zeta) &= \frac{2l+1}{\pi}\int_{S^2} e^{im\phi'} d^l_{mn}(\theta') && (97)\\
&\quad \times c_{-n}(k_0; r_1 e_3, r_2 e^{\varphi R(e_2)} e_3) \sin\theta' d\theta' d\phi' && (98)\\
&= \frac{2l+1}{\pi}\int_{S^2} e^{im\phi'} d^l_{mn}(\theta') \\
&\quad \times \sum_{j=|n|}^{\infty} \rho^j c_{\frac{j+n}{2},\frac{j-n}{2}}(k_0; r_1, \xi_3) \sin\theta' d\theta' d\phi' && (99)\\
&= \frac{2l+1}{\pi}\sum_{j=|n|}^{\infty} \rho^j \tilde{c}_{mn,\frac{j-n}{2},\frac{j+n}{2}}(r_1, \xi_3) && (100)
\end{aligned}
$$

The $\tilde{c}_{mn}$ are the outcome of the integration of $c_{\frac{j+n}{2},\frac{j-n}{2}}$ over θ' and ϕ'. Hence the expansion of f is;

$$
\begin{aligned}
f(g\zeta) &= \sum_{l=0}^{\infty}\sum_{|m|,|n|\leq l} \mathcal{D}^l_{mn}(g)(P^l_{nm}f)(\zeta) && (101)\\
&= \frac{2l+1}{\pi}\sum_{l=0}^{\infty}\sum_{|m|,|n|\leq l} \mathcal{D}^l_{mn}(g) \\
&\quad \times \sum_{j=|n|}^{\infty} \rho^j \tilde{c}_{mn,\frac{j-n}{2},\frac{j+n}{2}}(r_1, \xi_3) && (102)
\end{aligned}
$$

This gives a boundary condition on wave function in the sense that when expanded into power series, the function starts with the power $\rho^{|n|}$. As a side note, it must be stressed that an increase of $|n|$ by one corresponds to a doulbe increase in j, which is in consistent with the result given in the reference [2].

The associated vector bundle

$$E_l = \dot{X}_0 \times_l \mathcal{H}^l \qquad (103)$$

defined through (18) has a local structure $U \times \mathcal{H}^l$. We recall that the equivariant functions defined in (62) is in one to one correspondence with local sections in the associated vector bundle. From (62), we know that at the colinear configuration, the all but one components of $E^l_m f$ vanishes. This means the sections for the corresponding

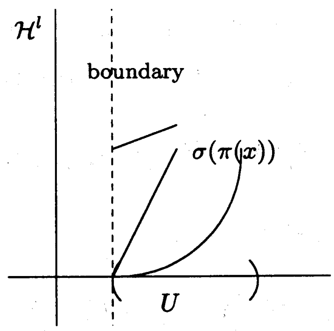

Figure 5: Sketch graphs show components of a local section in the associated fiber bundle. In the open set containing the boundary of $\dot{X}$, all but one components of the section tend to zero as they approach the boundary. For different components, the decay speed is dependent on its corresponding angular momentum value.

equivariant functions must approach zero, because they are continuous. In other words, towards the singular configuration, all (apart from the one which corresponds to $n = 0$) components of the section must somehow decay to zero. How they decay can be seen from the power series expansion in (100). The bigger the $|n|$, the faster the decay.

4.3 Remark

If we let $\zeta \longrightarrow \zeta_0$ (corresponds to $\varphi \longrightarrow 0$ or π), then $\xi_3 \longrightarrow r_2$ and $\rho \longrightarrow 0$, so that the terms of the right-hand side of $U(k_0^{-1})f$ vanish if $n' \neq 0$:

$$(U(k_0^{-1})f)(r_1\mathbf{e}_3, r_2 e^{\psi R(\mathbf{e}_3)} e^{\varphi R(\mathbf{e}_2)}\mathbf{e}_3)$$

$$= \sum_{n'=-\infty}^{\infty} e^{in'\psi'} \sum_{j=|n'|}^{\infty} \rho^j c_{\frac{j+n'}{2},\frac{j-n'}{2}}(k_0; r_1, \xi_3) \tag{104}$$

$$\longrightarrow c_{0,0}(k_0; r_1, \xi_3). \tag{105}$$

This implies further that;

$$(P^l_{nm}f)(\zeta_0) = 0 \quad \text{if} \quad n \neq 0, \tag{106}$$

which gives the result that is consistent with the one derived in (77).

5 Collision Singularity

In section 4, we discussed one type of singularity, that is when the particles are aligned in a straight line. Here we consider the case when all three particles collide at the origin.

Let $(r_1, r_2) = (0,0)$. Then the corresponding end of section is $\zeta_0 = (0,0)$. We recall that (70) holds for any ζ and any $g \in SO(3)$. Therefore we have for $g \in G_{\zeta_0} \cong SO(3)$

$$(E^l_m f)(0) = \mathcal{D}^l(g)(E^l_m f)(0). \tag{107}$$

This in terms of the local coordinates gives

$$(P^l_{nm} f)(0) = e^{-in\phi'} \sum_{|n'|\le l} d^l_{nn'}(\theta') e^{-in'\psi'} (P^l_{nm} f)(0), \tag{108}$$

and this holds for all θ', ψ', ϕ'. (107) says that the linear subspace spanned by $E^l_m f$ is invariant. Noting that $\mathcal{D}^l_m$ is a irreducible representation, we conclude that

$$(E^l_m f)(0) = 0, \qquad l \neq 0. \tag{109}$$

For $l = 0$ we simply have the identity equation since $\mathcal{D}^l = 1$. The implication of this is that in general we can not say that the wavefunction is zero, and therefore as a consequence of this, there is a possible collision after all. The whole purpose of this is to try to express the wavefunction as a Fourier expansion. The wavefunction which is expanded at the point 0 is

$$\begin{aligned} f(0) &= \sum_{l=0}^{\infty} \sum_{|m|,|n|\le l} \mathcal{D}^l_{mn}(g)(P^l_{nm} f)(0) && (110) \\ &= (P^0_{0,0} f)(0). && (111) \end{aligned}$$

5.1 Configuration in nbd of the collision

Since the center of mass of the system is fixed at the origin, we must have $\boldsymbol{x}_1 = \boldsymbol{x}_2 = \boldsymbol{x}_3 = 0$ when the collision takes place. In terms of Jacobi vectors (21–22), this corresponds to $\boldsymbol{r}_1 = \boldsymbol{r}_2 = 0$. The colliding configuration corresponds to $\eta_1 = \eta_2 = \eta_3 = 0$ in terms of the internal local coordinates. There is no reason why we can not expand the wavefunction in terms of $\mathcal{D}^l$ as before. The boundary of the shape space M is two dimensional, as opposed to three for the interior. However it is not always wise to think that there is a drop in the number of variables. Instead, here we simply see the triple collision situation as the special case—the case that some variables become insignificant. As already discussed, the configuration space for the triatomic system is six dimensional, and we revert our discussion back on the wavefunction $f(\boldsymbol{\alpha}, \boldsymbol{\beta})$ on

$\mathbb{R}^3 \times \mathbb{R}^3$, where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ really are nothing other than the Jacobi vectors (21–22). Each $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ have components α_j, and β_j, $j = 1, 2, 3$ respectively. Now, if this wavefunction is analytic at the origin, and therefore analytic when triple collision takes place, f has the expansion of the form

$$f(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \sum_{I,J} c_{IJ} \alpha^I \beta^J, \tag{112}$$

where we have used the notations

$$I = (i_1, i_2, i_3), \quad J = (j_1, j_2, j_3), \quad \alpha^I = \alpha_1^{i_1} \alpha_2^{i_2} \alpha_3^{i_3}, \quad \beta^J = \beta_1^{j_1} \beta_2^{j_2} \beta_3^{j_3}. \tag{113}$$

Here we emphasize once again that, for given f we would like to expand this series into a Fourier series in terms of the $\mathcal{D}$-functions. First we consider a section just as we did for the colinear case. We have already discussed that

$$M := X_0/SO(3) \cong \mathbb{R}^3 \times \mathbb{R}^3/SO(3) \tag{114}$$

is the shape space which is homeomorphic with $\{x \in \mathbb{R}^3 \mid x_3 \geq 0\}$. For π defined in (14) and for an open set $U \subset M$, we may express any $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \pi^{-1}(U)$ as

$$(\boldsymbol{\alpha}, \boldsymbol{\beta}) = g\sigma = (g\boldsymbol{\sigma_1}(q), \boldsymbol{\sigma_2}(q)), \qquad q \in U \tag{115}$$

where q are the local coordinates in M, $g \in SO(3)$, and $\boldsymbol{\sigma_j}$ are the components of σ defined in (16).

Let $P^n(\mathbb{R}^3 \times \mathbb{R}^3)$ be the space of homogeneous polynomials of degree n in α_i, β_j. Then we see that it is invariant under the $SO(3)$ action, which means that $SO(3)$ is represented in $P^n(\mathbb{R}^3 \times \mathbb{R}^3)$. This implies that the space $P^n(\mathbb{R}^3 \times \mathbb{R}^3)$ will be decomposed into irreducible subspaces with respect to the $SO(3)$ action. In each irreducible subspace, the basis polynomial transformation is subject to

$$p_m(g^{-1}\boldsymbol{\alpha}, g^{-1}\boldsymbol{\beta}) = \sum_{|n| \leq l} p_n(\boldsymbol{\alpha}, \boldsymbol{\beta}) \mathcal{D}^l_{nm}(g). \tag{116}$$

Hence if we substitute (115) into (112), we expect to be able to put f into a Fourier series in terms of $\mathcal{D}$-functions

$$f(g\boldsymbol{\sigma}_1(q), g\boldsymbol{\sigma}_2(q)) = \sum_{l=0}^{\infty} \sum_{|m|,|n| \leq l} \mathcal{D}^l_{mn}(g^{-1}) c^{(l)}_{mn}(q). \tag{117}$$

5.2 Decomposition of space of homogeneous polynomials

It is of our interest to investigate this Fourier series in detail. Let $P^n(\mathbb{R}^3)$ denote the space of homogeneous polynomials in $u_j, j = 1,2,3$. Then $P^n(\mathbb{R}^3)$ is decomposed into

$$P^n(\mathbb{R}^3) = H^n(\mathbb{R}^3) \oplus r^2 H^{n-2}(\mathbb{R}^3) \oplus \cdots \oplus \begin{cases} r^n H^0(\mathbb{R}^3) & \text{if } n \text{ is even} \\ r^{n-1} H^1(\mathbb{R}^3) & \text{if } n \text{ is odd} \end{cases} \tag{118}$$

where $H^n(\mathbb{R}^3)$ is the space of solid harmonics of degree n. Here we point out that it is isomorphic with the $(2n+1)$-dimensional space $\mathcal{H}^n$ for unitary irreducible representations of $SO(3)$. In addition to that r^2 is invariant under $g \in SO(3)$, the decomposition (118) is reduced to

$$P^n(\mathbb{R}^3) \cong \mathcal{H}^n \oplus \mathcal{H}^{n-1} \oplus \cdots \oplus \begin{cases} \mathcal{H}^0 & \text{if } n \text{ is even} \\ \mathcal{H}^1 & \text{if } n \text{ is odd} \end{cases} . \tag{119}$$

Therefore this decomposition applied to $P^l(\mathbb{R}^3 \times \mathbb{R}^3)$ gives

$$\begin{aligned} P^l(\mathbb{R}^3 \times \mathbb{R}^3) &= \sum_{n+m=l} H^n(\mathbb{R}^3_\alpha) \otimes H^m(\mathbb{R}^3_\beta) \\ &\oplus \sum_{n+m=l} H^n(\mathbb{R}^3_\alpha) \otimes |\beta|^2 H^{m-2}(\mathbb{R}^3_\beta) \\ &\oplus \sum_{n+m=l} |\alpha|^2 H^{n-2}(\mathbb{R}^3_\alpha) \otimes H^m(\mathbb{R}^3_\beta) \oplus \cdots \end{aligned} \tag{120}$$

where we have used the identity

$$P^l(\mathbb{R}^3 \times \mathbb{R}^3) = \sum_{n+m=l} P^n(\mathbb{R}^3) \otimes P^m(\mathbb{R}^3), \tag{121}$$

and the greek subscripts are placed so that one may not confuse the two $\mathbb{R}^3$'s. This should further be put in terms of $\mathcal{H}^n$'s;

$$\begin{aligned} P^l(\mathbb{R}^3 \times \mathbb{R}^3) &\cong \sum_{n+m=l} \mathcal{H}^n \otimes \mathcal{H}^m \\ &\oplus \sum_{n+m=l} \mathcal{H}^n \otimes \mathcal{H}^{m-2} \\ &\oplus \sum_{n+m=l} \mathcal{H}^{n-2} \otimes \mathcal{H}^m \oplus \cdots . \end{aligned} \tag{122}$$

We can again decompose (122) further, if we apply the *Clebsch-Gordan decomposition formula* for $SO(3)$,

$$\mathcal{H}^p \otimes \mathcal{H}^q \cong \mathcal{H}^{|p-q|} \oplus \mathcal{H}^{|p-q|+1} \oplus \cdots \oplus \mathcal{H}^{p+q} \tag{123}$$

and we finally obtain the decomposition

$$P^l(\mathbb{R}^3 \times \mathbb{R}^3) \cong \mathcal{H}^l \oplus \mathcal{H}^{l-1} \oplus 2\mathcal{H}^{l-2} \oplus \cdots . \tag{124}$$

5.3 Implication of the decomposition

We may deduce the main result of the article from the decomposition (124). The decomposition implies that $P^l(\mathbb{R}^3 \times \mathbb{R}^3)$ includes representations spaces $\mathcal{H}^m$ with $m \leq l$ only. Therefore the representation space $\mathcal{H}^n$ arise from $P^n(\mathbb{R}^3 \times \mathbb{R}^3)$ with $n \geq l$. Basis polynomials in $\mathcal{H}^n$ are subject to the transformation (116).

Now suppose that the wavefunction f is analytic at the origin. Given that we have a triatomic system, and if f is an eigenstate associated with the eigenvalue $l(l+1)$ of the total angular momentum operator $\boldsymbol{L}^2$, f must be a linear combination of $\mathcal{D}^l_{mn}(g)$, coefficients of which are expressed as power series in the local coordinates q. This implies that the eigenstate f expressed as a power series in α_i, β_j must have the lowest order terms of the form $\boldsymbol{\alpha}^I \boldsymbol{\beta}^J$ with $|I| + |J| = l$, where $|I| = i_i + i_2 + i_3$, and $|J| = j_1 + j_2 + j_3$.

5.4 Example

In order to justify the main result obtained in the previous subsection, we present an example here. Here we pay particular attention to the fact that the representation spaces of $SO(3)$, $P^1(\mathbb{R}^3)$, and $\mathcal{H}^1$ are isomorphic, and we consider the tensor product

$$P^1(\mathbb{R}^3) \times P^1(\mathbb{R}^3) = \{\mathrm{tr}(C^T \boldsymbol{\alpha}\boldsymbol{\beta}T) = \sum_{i,j} C_{ij}\alpha_i\beta_j \mid C \in \mathbb{C}^{3\times 3}\}. \tag{125}$$

The Clebsch-Gordan formula applied on this gives

$$\mathcal{H}^1 \otimes \mathcal{H}^1 \cong \mathcal{H}^0 \oplus \mathcal{H}^1 \oplus \mathcal{H}^2, \tag{126}$$

and here we aim to identify each component in the right hand side of (126). Just as we considered the basis of tensor product like the one in (116), here we consider the transformation of the basis $\boldsymbol{\alpha}\boldsymbol{\beta}^T$. This transformation is subject to

$$\boldsymbol{\alpha}\boldsymbol{\beta}^T \mapsto g(\boldsymbol{\alpha}\boldsymbol{\beta}^T)g^{-1} \tag{127}$$

then one has $\mathrm{tr}(C^T)g(\boldsymbol{\alpha}\boldsymbol{\beta}^T)g^{-1}) = \mathrm{tr}(gCg^{-1}\boldsymbol{\alpha}\boldsymbol{\beta}^T)$. So the transformation of C is subject to

$$C \mapsto A_g := gCg^{-1}. \tag{128}$$

Here we note that the symmetric and anti-symmetric matrices are invariant under the adjoint action of g, and since $\mathrm{tr}(g^{-1}Cg) = \mathrm{tr}(C)$, the representation of $SO(3)$ in $\mathbb{C}^{3\times 3}$ is reducible down to three subspaces

$$\mathbb{C}_0^{3\times 3} := \{\lambda I_3 \mid \lambda \in \mathbb{C}\} \tag{129}$$
$$\mathbb{C}_1^{3\times 3} := \{C \in \mathbb{C}^{3\times 3} \mid C = -C^T\} \tag{130}$$
$$\mathbb{C}_2^{3\times 3} := \{C \in \mathbb{C}^{3\times 3} \mid C = C^T, \mathrm{tr}(C) = 0\}. \tag{131}$$

It is trivial to observe that $\dim \mathbb{C}_0^{3\times 3} = 1$, $\dim \mathbb{C}_1^{3\times 3} = 3$, $\dim \mathbb{C}_2^{3\times 3} = 5$, and $\mathbb{C}^{3\times 3} = \bigoplus_{j=0}^{3} \mathbb{C}_j^{3\times 3}$, so we may identify $\mathbb{C}_j^{3\times 3}$ with $\mathcal{H}^j$.

For $C_1, C_2 \in \mathbb{C}^{3\times 3}$, define the inner product

$$\langle C_1, C_2 \rangle = \mathrm{tr}(C_1^* C_2), \tag{132}$$

and under this inner product, it can be shown easily that the adjoint operator A_g is unitary. Recall that $\mathbb{C}_j^{3\times 3}$ are invariant subspaces of $\mathbb{C}^{3\times 3}$ under A_g, we observe that the adjoint operator restricted to $\mathbb{C}_j^{3\times 3}$ domain is a $U(2j+1)$ operator. Further, note that $\bigoplus_{j=0}^{3} \mathbb{C}_j^{3\times 3}$ is an orthogonal direct sum. In particular, if we choose C_1 and C_2 such that $C_1^T = -C_1$, $C_2^T = C_2$, we have

$$\langle C_1, C_2 \rangle = 0 \tag{133}$$

and this implies that $\mathbb{C}_0^{3\times 3} \oplus \mathbb{C}_2^{3\times 3}$ and $\mathbb{C}_1^{3\times 3}$ are orthogonal to each other. In addition, if we particularly choose $C_1 = \lambda I_3$ and C_2 with $\mathrm{tr}(C_2) = 0$, we again have (133), implying $\mathbb{C}_0^{3\times 3}$ and $\mathbb{C}_2^{3\times 3}$ are orthogonal to each other.

The bases of $\mathcal{H}^0$ and $\mathcal{H}^1$ are $\boldsymbol{\alpha} \cdot \boldsymbol{\beta}$ and the components of $\boldsymbol{\alpha} \times \boldsymbol{\beta}$ respectively. The bases of $\mathcal{H}^2$ are $\alpha_i\beta_j + \alpha_j\beta_i (i < j)$, $\alpha_1\beta_1 - \alpha_2\beta_2$, $\alpha_2\beta_2 - \alpha_3\beta_3$. However, these bases should be transformed into suitable ones in order to get unitary matrices $\mathcal{D}^l(g), l = 1, 2$ as transformation matrices such that (116) holds.

For the case $l = 1$, let $\boldsymbol{\gamma} = \boldsymbol{\alpha} \times \boldsymbol{\beta}$. If $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are transformed to $g\boldsymbol{\alpha}$ and $g\boldsymbol{\beta}$ respectively, then $\boldsymbol{\gamma}$ transforms subject to $\boldsymbol{\gamma} \mapsto g\boldsymbol{\gamma}$, and we have

$$p_n^{(1)}(g^{-1}\gamma) = \sum_m p_m^{(1)}(\gamma)\mathcal{D}^1_{mn}(g) \tag{134}$$

for the polynomials defined by

$$(p_1^{(1)}, p_0^{(1)}, p_{-1}^{(1)}) = \left(-\frac{\gamma_1 + i\gamma_2}{\sqrt{2}}, \gamma_3, \frac{\gamma_1 - i\gamma_2}{\sqrt{2}}\right). \tag{135}$$

In fact the polynomials $p_m^{(1)}$ are related to the spherical harmonics by

$$p_m^{(1)}(\boldsymbol{u}) = \sqrt{\frac{4\pi}{3}} rY_{1m}(\theta, \phi), \qquad m = -1, 0, 1. \tag{136}$$

Next is the case when $l = 2$. First note that

$$\mathcal{H}^2 \cong H^2(\mathbb{R}^3) = \{\mathrm{tr}(C^T\boldsymbol{u}\boldsymbol{u}^T) = \sum_{i,j} C_{ij}u_iu_j \mid C \in \mathbb{C}^{3\times3}, C = C^T, \mathrm{tr}(C) = 0\}, \tag{137}$$

and we present the following as the bases of $H^2(\mathbb{R}^3)$;

$$q_{-2} = (u - iv)^2/2, \tag{138}$$
$$q_{-2} = w(u - iv), \tag{139}$$
$$q_0 = (2w^2 - (u^2 + v^2)), \tag{140}$$
$$q_1 = -w(u + iv) \tag{141}$$
$$q_2 = (u + iv)^2/2. \tag{142}$$

Similarly these polynomials are related to the spherical harmonics by

$$q_m(\boldsymbol{u}) = \sqrt{\frac{8\pi}{15}} r^2Y_{2m}(\theta, \phi), \qquad m = 2, 1, 0, -1, -2 \tag{143}$$

that transform subject to

$$q_m(g^{-1}) = \sum_m q_n(\boldsymbol{u})\mathcal{D}^2_{nm}(g). \tag{144}$$

For the bases

$$\sigma_{-2} = \tfrac{1}{2}\begin{pmatrix} 1 & -i & 0 \\ -i & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \sigma_{-1} = \tfrac{1}{2}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & -i \\ 1 & -i & 0 \end{pmatrix}, \quad \sigma_0 = \tfrac{1}{\sqrt{6}}\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix},$$
$$\sigma_1 = \tfrac{1}{2}\begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -i \\ -1 & -i & 0 \end{pmatrix}, \quad \sigma_2 = \tfrac{1}{2}\begin{pmatrix} 1 & i & 0 \\ i & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{145}$$

for $\mathbb{C}_2^{3\times 3}$, the solid harmonics $q_m(\boldsymbol{u})$ is put in the form

$$q_m(\boldsymbol{u}) = \mathrm{tr}(\sigma_m \boldsymbol{u}\boldsymbol{u}^T), \qquad m = -2, -1, 0, 1, 2, \tag{146}$$

and the $q_m(\boldsymbol{u})$ have the generating function

$$Q_2(\boldsymbol{u}, t) = \sum_{-2}^{2} c_m q_m(\boldsymbol{u}) t^{2-m} \tag{147}$$

with $(c_{-2}, c_{-1}, c_0, c_1, c_2) = (2, 4, 2\sqrt{6}, 4, 2)$. If we observe that Q_2 is expressed as

$$Q_2(\boldsymbol{u}, t) = (\sqrt{2}p_{-1}^{(1)}(\boldsymbol{u})t^2 + 2p_0^{(1)}(\boldsymbol{u})t + \sqrt{2}p_1^{(1)}(\boldsymbol{u}))^2, \tag{148}$$

we find that

$$q_{-2}(\boldsymbol{u}) = p_{-1}^{(1)}(\boldsymbol{u})^2, \tag{149}$$
$$q_{-1}(\boldsymbol{u}) = \sqrt{2}p_0^{(1)}(\boldsymbol{u})p_{-1}^{(1)}(\boldsymbol{u}), \tag{150}$$
$$q_0(\boldsymbol{u}) = \frac{2}{\sqrt{6}}(p_0^{(1)}(\boldsymbol{u}^2 + p_1^{(1)}(\boldsymbol{u})p_{-1}^{(1)}(\boldsymbol{u})), \tag{151}$$
$$q_1(\boldsymbol{u}) = \sqrt{2}p_0^{(1)}(\boldsymbol{u})p_1^{(1)}(\boldsymbol{u}), \tag{152}$$
$$q_2(\boldsymbol{u}) = p_1^{(1)}(\boldsymbol{u})^2. \tag{153}$$

Further, define the function

$$P_2(\boldsymbol{\alpha}, \boldsymbol{\beta}, t) = ((\alpha_1 - i\alpha_2)t^2 + 2\alpha_3 t - (\alpha_1 + \alpha_2))((\beta_1 - i\beta_2)t^2 + 2\beta_3 t - (\beta_1 + i\beta_2)), \tag{154}$$

which expands into

$$P_2(\boldsymbol{\alpha}, \boldsymbol{\beta}, t) = \sum_{-2}^{2} c_m p_m(\boldsymbol{\alpha}, \boldsymbol{\beta}) t^{2-m}, \tag{155}$$

$$p_{-2}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{2}(\alpha_1 - i\alpha_2)(\beta_1 - i\beta_2), \tag{156}$$
$$p_{-1}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{2}(\alpha_3(\beta_1 - i\beta_2) + (\alpha_1 - i\alpha_2)\beta_3), \tag{157}$$
$$p_0(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{2\sqrt{6}}(4\alpha_3\beta_3 - (\alpha_1 - i\alpha_2)(\beta_1 + i\beta_2) - (\alpha_1 + i\alpha_2)(\beta_1 - i\beta_2)), \tag{158}$$
$$p_1(\boldsymbol{\alpha},\boldsymbol{\beta}) = -\frac{1}{2}((\alpha_1 + i\alpha_2)\beta_3 + \alpha_3(\beta_1 + i\beta_2)), \tag{159}$$
$$p_2(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{2}(\alpha_1 + i\alpha_2)(\beta_1 + i\beta_2). \tag{160}$$

The relations with $p_m^{(1)}$ are given by

$$p_{-2}(\boldsymbol{\alpha},\boldsymbol{\beta}) = p_{-1}^{(1)}(\boldsymbol{\alpha})p_{-1}^{(1)}(\boldsymbol{\beta}), \tag{161}$$
$$p_{-1}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{\sqrt{2}}{2}(p_0^{(1)}(\boldsymbol{\alpha})p_{-1}^{(1)}(\boldsymbol{\beta}) + p_{-1}^{(1)}(\boldsymbol{\alpha})p_0^{(1)}(\boldsymbol{\beta}), \tag{162}$$
$$p_0(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{\sqrt{6}}(2p_0^{(1)}(\boldsymbol{\alpha})p_0^{(1)}(\boldsymbol{\beta}) + p_{-1}^{(1)}(\boldsymbol{\alpha})p_1^{(1)}(\boldsymbol{\beta}) + p_1^{(1)}(\boldsymbol{\alpha})p_{-1}^{(1)}(\boldsymbol{\beta}) \tag{163}$$
$$p_1(\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{\sqrt{2}}{2}(p_1^{(1)}(\boldsymbol{\alpha})p_0^{(1)}(\boldsymbol{\beta}) + p_0^{(1)}(\boldsymbol{\alpha})p_1^{(1)}(\boldsymbol{\beta})), \tag{164}$$
$$p_2(\boldsymbol{\alpha},\boldsymbol{\beta}) = p_1^{(1)}(\boldsymbol{\alpha})p_1^{(1)}(\boldsymbol{\beta}) \tag{165}$$

The functions $p_m(\boldsymbol{\alpha},\boldsymbol{\beta})$ form a basis of the space of polynomials associated with $\mathbb{C}_2^{3\times 3}$;

$$\{\mathrm{tr}(C^T\boldsymbol{\alpha}\boldsymbol{\beta}) = \sum_{i,j} C_{ij}\alpha_i\beta_j \mid C = C^T, \mathrm{tr}(C) = 0\} \tag{166}$$

and are expressed as

$$p_m(\boldsymbol{\alpha},\boldsymbol{\beta}) = \mathrm{tr}(\sigma_m\boldsymbol{\alpha}\boldsymbol{\beta}). \tag{167}$$

Here we note that $q_m(\boldsymbol{u})$ transforms according to $q_m(g^{-1}\boldsymbol{u}) = \sum_n q_n(\boldsymbol{u})\mathcal{D}_{nm}^2(g)$. Since $q_m(g^{-1}\boldsymbol{u} = \mathrm{tr}(g\sigma_m g^{-1}\boldsymbol{u}\boldsymbol{u}^T)$, and since $\sum_n q_n(\boldsymbol{u})\mathcal{D}_{nm}^2(g) = \mathrm{tr}(\sum_n \sigma_n\mathcal{D}_{nm}^2(g)\boldsymbol{u}\boldsymbol{u}^T)$, we see that σ_m are subject to the transformation

$$A_g\sigma_m = \sum_n \sigma_n\mathcal{D}_{nm}^2(g). \tag{168}$$

If we apply this transformation rule to $p_m(\boldsymbol{\alpha}, \boldsymbol{\beta})$, we find that

$$p_m(g^{-1}\boldsymbol{\beta}, g^{-1}\boldsymbol{\beta}) = \sum_n p_n(\boldsymbol{\alpha}, \boldsymbol{\beta})\mathcal{D}^2_{nm}(g). \qquad (169)$$

Therefore we found a realization of the component space $\mathcal{H}^2$ in the decomposition (126).

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