REVISTA DE LA ESCUELA DE FÍSICA
• Vol. VI, No. 1 • ISSN 2412-2564

Un sistema cuántico que gira sin momento angular y sin cambios en su forma

A rotating quantum system without angular momentum and shape deformations

E. SERRANO-ENSÁSTIGA[1]

Recibido: 24 abril de 2018 / Aceptado: 3 de junio de 2018

[1]Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Apartado Postal 70-543, Ciudad de México 04510, México. email: eduardo.serrano-ensastiga@uni-tuebingen.de

Agradecimientos

El autor le agradece a Daniel Flores por la invitación a publicar en la Rev. Esc. Fis.

Especial Thanks

The author thanks to Daniel Flores for the invitation to publish in the Rev. Esc. Fis. journal.

La dinámica independiente de traslaciones de un sistema cuántico de n cuerpos tiene muchas aplicaciones, e.g., en sistemas moleculares y nucleares, donde es común clasificar los grados de libertad del sistema en 3 rotacionales y $3n-6$ coordenadas de forma. Es sabido que existe una interacción entre los grados rotacionales y de forma. En particular, cambios en la forma pueden llegar a inducir un cambio en la orientación del sistema. En este trabajo, mostramos un sistema cuántico que gira pero sin deformar su densidad de probabilidades de forma y con momento angular cero. El cambio de la orientación es monitoreada con una función de onda de orientaciones localizada. Caracterizamos estas funciones de onda localizados y estudiamos su evolución bajo un Hamiltoniano tipo rotor rígido, concluyendo que esta clase de funciones de onda pueden rotar, independientes de su evolución de formas.

The free translational dynamics of an n-body quantum system has many applications, e.g. in molecular and nuclei systems, where it is common to classify the degrees of freedom of the system in 3 rotational and $3n-6$ shape coordinates. It is known that there exists an interaction between the shape and orientation degrees of freedom. In particular, changes of the shape could induce an orientation change. In this work, it is shown a rotating quantum system which does not deform its shape probability density and with vanishing angular momentum. The orientation change is monitored with a localized orientation wavefunction. We characterize the localized wavefunctions and study their evolution under a rigid rotor-like Hamiltonian, concluding that this kind of wavefunctions may rotate by their own.

PALABRAS CLAVES

Métodos Geométricos, Problema de N Cuerpos, Control Cuántico,Movimiento Rotacional

KEYWORDS

Geometric Methods, *N* Body Problem, Quantum Control,Rotational Motion

PACS

02.40.-k, 03.64.-w, 33.20.Wr, 36.20.Ng

I | INTRODUCTION

A system of n isolating point particles has $3n$ coordinates separated in three coordinates of the center of mass position, three of the orientation of the system and $3n-6$ to describe the shape of the system. The last coordinates are related to the vibrational modes in small oscillations. The orientation and shape coordinates do not evolve independently in the most of the physical systems producing many phenomena, *e.g.*, the falling cat problem (Kane & Scher, 1969; Montgomery, 1993), the re-orientation of a diver (Frolich, 1979), or the rovibrational excitations of molecules (Mitchell & Littlejohn, 1999; Ovchinnikov, Erikhman, & Pronin, 2001).

The emergence of geometrical methods in the study of the n-body problem, pioneered by Guichardet (Guichardet, 1984), have provided extensions of the subject, in particular in the interplay between orientation and shape dynamics (Shapere & Wilczek, 1989; Tachibana & Iwai, 1986) The quantum version of the problem has also been benefited by these approaches, leading to new advances in the theory and its potential applications in molecular dynamics (Littlejohn, Mitchell, Reinsch, Aquilanti, & Cavalli, 1998a, 1998b; Littlejohn & Reinsch, 1997; Mitchell & Littlejohn, 2000).

Nowadays scientists have found and synthesized machine-like molecules (Kottas, Clarke, Horinek, & Michl, 2005; Ohmann, 2015; Perera, 2013), *i.e.*, molecules managing a particular motion with operable degrees of freedom. The molecules are described in a semi-classical way because the considered constituent parts are too big to have a purely quantum behavior. These and incoming systems may present orientation-shape dynamics with new phenomena given by their quantum nature. For instance, the quantum version of the falling cat problem (Chryssomalakos, Hernández-Coronado, & Serrano-Ensástiga, 2015) may represent the dynamics of the constituent atoms of a molecule.

The aim of the paper is the presentation of quantum systems which, counter-intuitive to our (classical) experience, rotate with vanishing angular momentum expectation value and invariant (quantum) shape. The examples are made with the three-body system. The outline of this paper is as follows: Sec. II reviews the classic n-body problem, following closely (Littlejohn & Reinsch, 1997). In Sec. III is presented the three-body model and an example of a system which rotates under a cyclic shape deformation and with vanishing total angular momentum. Sec. IV reviews the quantum version of the n-body problem and the approximations used in this work. The three-body quantum system and our counter-intuitive examples are presented in Sec. V. Conclusions are summarized in Sec. VI.

II | CLASSICAL CASE

The first step is to consider a body consisting of n point-like particles with an interacting potential V and no other external force. The Lagrangian of the system is

$$L = \frac{1}{2}\sum_{\alpha=1}^{n} |\dot{\mathbf{r}}_{s\alpha}|^2 + V(\mathbf{r}_{s\alpha}), \tag{1}$$

where $\mathbf{r}_{s\alpha}$ is the α-th particle's position vector with respect to a fixed inertial frame called the *space frame*. The absence of external forces suggests the factorization of the center of mass dynamics writing the Lagrangian with relative vectors, *e.g.*, the mass-weighted Jacobi vectors,

$$\rho_{s\alpha} = \sqrt{\mu_\alpha}\sum_{\beta=1}^{N} T_{\alpha\beta}\mathbf{r}_{s\beta}, \quad \alpha = 1,\ldots,n-1 \tag{2}$$

where μ_α are the reduced masses and T is a numerical matrix (see (Littlejohn & Reinsch, 1997) for more details) such that the vectors $\rho_{s\alpha}$ are invariant under translations. Using the previous coordinate transformation, the Lagrangian takes the form

$$L = \frac{1}{2}M|\dot{\mathbf{R}}_s|^2 + \sum_{\alpha=1}^{n}|\dot{\rho}_{s\alpha}|^2 + V(\rho_{s\alpha}). \tag{3}$$

The configuration space of the whole system is $\mathbb{R}^{3n} = \mathbb{R}^3 \times \mathcal{C}$, where $\mathcal{C} = \mathbb{R}^{3n-3}$ is the translation-reduced configuration space. For the rest of the paper, $\mathbf{R}_s = \dot{\mathbf{R}}_s = 0$ and $\mathcal{C}$ is referred simply as the configuration space. A point in $\mathcal{C}$ specifies the shape and orientation of the body. Three degrees of freedom define the orientation system (for instance, the Euler angles) and there are $3n-6$ remaining coordinates q^μ which specify the body's shape, where q^μ are independent functions on $\mathcal{C}$ invariant under proper rotations,

$$q^\mu(\rho_{s,1},\ldots,\rho_{s,n-1}) = q^\mu(\mathsf{R}\rho_{s,1},\ldots,\mathsf{R}\rho_{s,n-1}), \tag{4}$$

for all $\mathsf{R} \in SO(3)$. To define the body's orientation operationally, on the other hand, we require (i) an orthonormal frame called the body frame, fixed to the body for each shape and given by the relations $\rho_\alpha = \rho_\alpha(q^\mu)$, $\alpha = 1,\ldots,n-1$, (the quantities referred to the body frame are written without the subindex s), and (ii) the rotation $\mathsf{R} \in SO(3)$ that maps the body frame to the space frame parametrized, for instance, by Euler angles $\mathsf{R} = \mathsf{R}(\theta^i)$. Fixing a body frame for each shape is a choice of gauge, that defines as reference orientation the one where the body and space frames coincide. The factorization of (non-collinear) configurations in "shape times orientation" leads to a description of $\mathcal{C}$ as a $SO(3)$ *principal fiber bundle* (Littlejohn & Reinsch, 1997; Nakahara, 1990) and its mathematical construction is as follows. We let $p \in \mathcal{C}$ be some specific configuration, and we consider the set of configurations given by the orbit of p under the action of $SO(3)$ $O_p = \mathsf{R}p|\mathsf{R} \in SO(3)$. The configurations of O_p have the same shape as p, and they form a surface in $\mathcal{C}$. The non-collinear configurations of the system have an orbit of dimension 3, each of which is a copy of $SO(3)$. The orbit of collinear configurations are a copy of the two-sphere S^2 , and when all the particles coincide in a single point p (an n-body collision), the orbit is just the point p itself; in this case the orbit is zero-dimensional. For systems with number of particles $n \geq 3$, the configurations without orbits diffeomorphic to $SO(3)$ is a set of measure zero. The *shape space* of $\mathcal{C}$ is the quotient space $\mathcal{S} = \mathcal{C}/SO(3)$, the space in which a single point represents a whole orbit, *i.e.*, the equivalence class of configurations of the same shape. If we exclude the configurations without orbit diffeomorphic to $SO(3)$, then the remaining configuration space qualifies properly speaking as a *principal fiber bundle*, in which the shape space is the base space, the *structure group* is $SO(3)$, and the fibers are the orbits. The whole configuration space $\mathcal{C}$ will be considered as a principal fiber bundle, just taking into account that there are points in the base space where the fiber *shrinks* and silly situations may occur. The total space $\mathcal{C}$ has a surjective projection map $\pi : \mathcal{C} \to \mathcal{S}$ mapping each point p of $\mathcal{C}$ to its equivalence class in $\mathcal{S}$. In the fiber-bundle picture, a choice of gauge is a locally smooth specification of a unique point in each fiber, *i.e.*, the graph of a continuous map $\sigma : S \to \mathcal{C}$ such that $\pi(\sigma(x)) = x$ for all $x \in \mathcal{S}$. The graph of σ, called a *section*, is a surface which cuts through the fibers, specifying the reference orientation for each shape configuration, *i.e.*, the body frame. This fiber bundle is in general non-trivial, so that a section cannot be chosen globally, *i.e.*, there is no smooth global assignment of a body frame covering the whole base space.
In terms of these orientation and shape coordinates, (θ^i, q^μ), and a section $\rho_\alpha(q^\mu)$ as above, a point $(\rho_{s,1},\ldots,\rho_{s,n-1})$ in $\mathcal{C}$ is defined by

$$\rho_{s,\alpha} = \mathsf{R}(\theta^i)\rho_\alpha(q^\mu), \quad \alpha = 1,\ldots,n-1. \tag{5}$$

The above relation expresses the fact that given a shape of the body q^μ , and a reference orientation $\rho_\alpha(q^\mu)$, any configuration of the body, with that shape, can be reached through a unique rotation $R(\theta^i)$. For the tangent space $T\mathcal{C}$, it will prove convenient to use an anholonomic basis, such that the velocity vector $\mathbf{v}$ of the system has components $v^a = (\omega, \dot{q}^\mu)$, where

$$\omega^i = -\frac{1}{2}\varepsilon^{ijk}(\mathsf{R}^T \cdot \dot{\mathsf{R}})_{jk}, \tag{6}$$

is the i-th component of the angular velocity of the body frame w.r.t. the space frame, referred to the body frame (as indicated by the absence of subscript s) — the corresponding basis vectors satisfy the $SO(3)$ Lie algebra. In the above expression, and in what follows, repeated indices are implicitly summed over and the Greek indices μ, ν represent shape coordinates.
The Lagrangian (3) can be written in the form

$$L = \frac{1}{2}G_{ab}\nu^a\nu^b - V(q), \quad (G_{ab}) \equiv \begin{pmatrix} \mathsf{M} & \mathsf{M}\mathbf{A}_\nu \\ \mathbf{A}_\nu^T\mathsf{M} & g_{\mu\nu} + \mathbf{A}_\mu \cdot \mathsf{M} \cdot \mathbf{A}_\nu \end{pmatrix}, \tag{7}$$

where (G_{ab}) is the metric in configuration space $\mathcal{C}$, defined by the kinetic energy, M is the inertia tensor, and

$$\begin{aligned} \mathbf{A}_\mu &= \mathsf{M}^{-1}\sum_{\alpha=1}^{n-1}\rho_\alpha \times \frac{\partial \rho_\alpha}{\partial q^\mu}, \\ g_{\mu\nu} &= \sum_{\alpha=1}^{n-1}\frac{\partial \rho_\alpha}{\partial q^\mu}\cdot\frac{\partial \rho_\alpha}{\partial q^\nu} - \mathbf{A}_\mu \cdot \mathsf{M} \cdot \mathbf{A}_\nu, \end{aligned} \tag{8}$$

are the Coriolis gauge potential and the metric on shape space $\mathcal{S}$, respectively.
A velocity vector of the form $v^a = (\omega, 0)$ is purely rotational, or *vertical*, since $\dot{q}^\mu = 0$ implies the body's shape is not changing. A complementary notion of horizontality is furnished by decreeing a velocity vector *horizontal* if the corresponding motion of the system has zero total angular momentum. It turns out that horizontal and vertical vectors are orthogonal according to the above metric G. In the anholonomic basis introduced earlier, the angular momentum referred to the body frame is given by

$$\mathbf{L} = \mathsf{M} \cdot (\omega + \mathbf{A}_\mu \dot{q}^\mu). \tag{9}$$

The total angular momentum in the space frame $\mathbf{L}_s$ is constant, which referred in the body frame is given by

$$\mathsf{R}^{-1}\mathbf{L}_s = \mathbf{L} = \mathsf{M} \cdot (\omega + \mathbf{A}_\mu \dot{q}^\mu), \tag{10}$$

The change of the frame R with respect to t is calculated with the previous equation,

$$\hat{\mathbf{n}}\, d\eta = \omega\, dt = \mathsf{M}^{-1}\mathbf{L}\, dt - \mathbf{A}_\mu dq^\mu, \tag{11}$$

where $\hat{\mathbf{n}}\, d\eta$ is an infinitesimal rotation of angle $d\eta$ around the axes $\hat{\mathbf{n}}$. When $\mathbf{L}_s = 0$, eq. (11) only depends of the curve in the shape space,

$$\mathsf{R}(t) = \mathcal{P}\exp\left(-\int_{q_0}^{q(t)} A_\mu dq^\mu\right), \tag{12}$$

where the body and space frame coincides at $t = 0$, $\mathcal{P}\exp$ is a path integral (the composition of rotations is non-Abelian), and A_μ is the antisymmetric matrix associated to the gauge potential, $(A_\mu)_{ij} = -\varepsilon_{ijk}A^k_\mu$. The rotation is independent of the gauge (and then it is a physical quantity) only for closed curves in the shape space. The equation (11) with $\mathbf{L} = 0$ is a connection in the principal fiber bundle, which defines a horizontal vector in each point of $\mathcal{C}$, such that for each curve in the base (shape) space $q(t)$, the connection gives the horizontal lift in $\mathcal{C}$ given by eq. (12). For $\mathbf{L} \neq 0$, the infinitesimal rotation (11) acquires an additional time-dependent contribution $(\mathsf{M}^{-1}\mathbf{L})dt$.

Just as in Yang-Mills gauge field theory, we define an associated curvature 2-form $\mathbf{B}$, called in this case the *Coriolis* tensor, with components given by

$$\mathbf{B}_{\mu\nu} = \partial_\mu \mathbf{A}_\nu - \partial_\nu \mathbf{A}_\mu - \mathbf{A}_\mu \times \mathbf{A}_\nu, \tag{13}$$

such that a cyclic deformation in shape space, with $\mathbf{L} = 0$, around the infinitesimal parallelogram spanned by the vectors y^μ and z^μ , produces the gauge-covariant infinitesimal rotation generated by $\omega dt = -\mathbf{B}_{\mu\nu}y^\mu z^\nu$. Note that $\mathsf{R} \neq 1$ requires both $\mathbf{B} \neq 0$ and a non-zero enclosed area by the closed path $q^\mu(t)$ in shape space.

The dynamics of the system can also be described by means of the gauge-covariant Hamiltonian

$$H = \frac{1}{2}\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L} + \frac{1}{2}(p_\mu - \mathbf{A}_\mu\cdot\mathbf{L})g^{\mu\nu}(p_\nu - \mathbf{A}_\nu\cdot\mathbf{L}) + V(q), \tag{14}$$

where $p_\mu = g_{\mu\nu}\dot{q}^\nu + \mathbf{A}_\mu\cdot\mathbf{L}$ is the momentum conjugate to the shape coordinate q^μ . The equation (10) is recovered using the Hamilton equations for a non-holonomic frame in eq. (14) (Littlejohn & Reinsch, 1997).

III | THREE- BODY SYSTEM

Let us consider three particles with masses $\{m_i\}_{i=3}^3$ and position vectors $\{r_s i\}_{i=1}^3$, respectively. We use the Jacobi vectors

$$\rho_{s1} = \sqrt{\mu_1}(\mathbf{r}_{s2} - \mathbf{r}_{s1}), \quad \rho_{s2} = \sqrt{\mu_2}(\mathbf{r}_{s3} - \mathsf{R}_{s,12}), \tag{15}$$

with

$$\mu_1 = \frac{m_1 m_2}{m_1 + m_2}, \quad \mu_2 = \frac{m_3(m_1+m_2)}{m_1+m_2+m_3}, \quad \mathsf{R}_{s,12} = \frac{m_1\mathbf{r}_{s1} + m_2\mathbf{r}_{s2}}{m_1+m_2} \tag{16}$$

where μ_j are the reduced masses of each particles' cluster and $\mathsf{R}_{s,12}$ is the center of mass of the particles 1 and 2. The following shape coordinates will allow us to write the Hamiltonian in a compact form,

$$q_1 = \rho_{s1}^2 - \rho_{s2}^2,\ q_2 = 2\rho_{s1}\cdot\rho_{s2},\ q_3 = 2|\rho_{s1}\times\rho_{s2}| \geq 0 \tag{17}$$

Fig. 1 shows the shape space, with the associated triangle shape for some particular points.

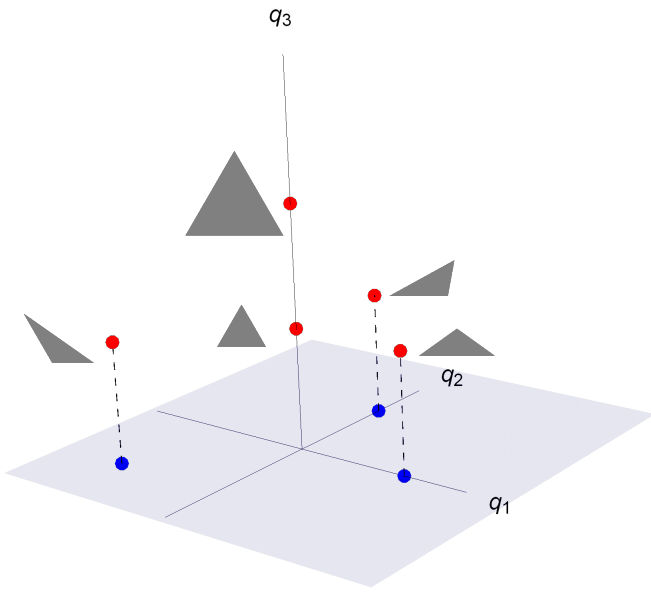

Figure 1: Shape space of the three-body system with equal masses. The gray triangles are the shapes of the system in the red points (q_1, q_2, q_3) =(0, 0, 1), (0, 0, 2), (1, 0, 1), (0, 1, 1), (1, 1, 1), respectively. The blue points and dashed lines remark the position of the red points.

We define for practical issues the variable, $q = \rho_{s1}^2 + \rho_{s2}^2 = (q_1^2 + q_2^2 + q_3^2)^{1/3}$. To the gauge, we use the so-called *north regular gauge* (Littlejohn & Reinsch, 1997).

$$\rho_1 = \frac{1}{2\sqrt{q+q_3}}(q+q_3+q_1, q_2, 0), \quad \rho_2 = \frac{1}{2\sqrt{q+q_3}}(q_2, q+q_3-q_1, 0) \tag{18}$$

This gauge has not a Dirac-like singularity (called in molecular physics an Iwai monopole (Iwai, 1987), a characteristic that other gauges have (Iwai, 1987; Tennyson & Sutcliffe, 1982). Now, we can calculate the quantities appeared in the Hamiltonian,

$$g^{\mu\nu} = 4q(dq_1^2 + dq_2^2 + dq_3^2), \quad \mathbf{A}_\mu dq^\mu = \frac{q_1 dq_2 - q_2 dq_1}{2q(q+q_3)}\hat{\mathbf{z}}. \tag{19}$$

$$M = \begin{pmatrix} \frac{q-q_1}{2} & -\frac{q_2}{2} & 0 \\ -\frac{q_2}{2} & \frac{q+q_1}{2} & 0 \\ 0 & 0 & q \end{pmatrix}, \quad M^{-1} = \begin{pmatrix} \frac{2(q+q_1)}{q_3^2} & \frac{2q_2}{q_3^2} & 0 \\ \frac{2q_2}{q_3^2} & \frac{2(q-q_1)}{q_3^2} & 0 \\ 0 & 0 & q^{-1} \end{pmatrix}. \tag{20}$$

Accordingly, the Hamiltonian (14) takes the form

$$H = \left(\frac{q+q_1}{q_2^2}\right)L_x^2 + \left(\frac{q-q_1}{q_3^2}\right)L_y^2 + \left(\frac{1}{q+q_3}\right)L_z^2 + \left(\frac{2q_2}{q_3^2}\right)L_xL_y - \frac{2L_z}{q+q_3}(-q_2p_1+q_1p_2) + 2q(p_1^2+p_2^2+p_3^2) + V(q). \tag{21}$$

1 | Rigid rotor case

In this case, the shape momentum p_μ is not proportional to q^u. For the rigid rotor case, $p_{mu} = \mathbf{A}_\mu \cdot \mathbf{L}$ and its Hamiltonian is

$$H = \frac{1}{2}L\cdot M^{-1} = \frac{(q+q_1)}{q_3^2}L_x^2 + \frac{(q-q_1)}{q_3^2}L_y^2 + \frac{2q_2}{q_3^2}L_xL_y + \frac{1}{2q}L_z^2 \tag{22}$$

The north regular gauge is not oriented to the principal axes in general, only when $q_2 = 0$. To get an intuition of the shape coordinates, we consider a three-body system with an isosceles triangle configuration and two particles of equal masses (see Fig. 2). The position vectors of the particles are

$$r_{s1} = \left(\frac{-a}{2}, -\frac{\sqrt{4b^2-a^2m}}{4M+2m}, 0\right), r_{s2} = \left(\frac{a}{2}, -\frac{\sqrt{4b^2-a^2m}}{4M+2m}, 0\right), r_{s3} = \left(0, \frac{\sqrt{4b^2-a^2m}}{4M+2m}, 0\right) \tag{23}$$

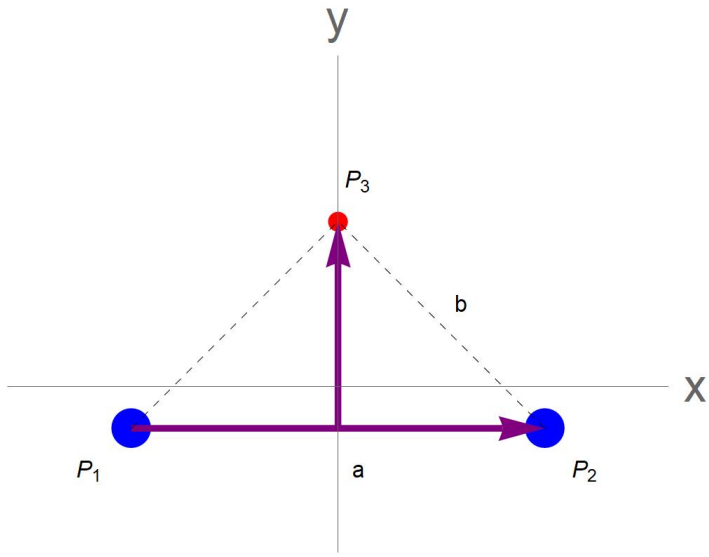

Figure 2: Three-body system with isosceles triangle configuration. The blue and red particles have masses M and m, respectively. The purple arrows are proportional to the weighted Jacobi vectors.

The shape coordinate q 2 = 0 and the inertia tensor is diagonal for this configuration class. Then, the coordinate system is in the principal axes of the system and the inertia moments are

$$I_x = \frac{mM(4b^2-a^2)}{2(2M+m)} = \frac{q_3^2}{2(q+q_1)}, I_y = \frac{Ma^2}{2} = \frac{q_3^2}{2(q-q_1)}, I_z = \frac{M(2mb^2+Ma^2}{2M+m} = q \tag{24}$$

The equilateral triangle configurations are in the q_3 axis, which are the unique configurations with a doubly degenerated inertia moment. The value of q_3 is proportional to the area. The collinear configurations are in the $q_1 - q_2$ plane.

2 | Vanishing total angular momentum

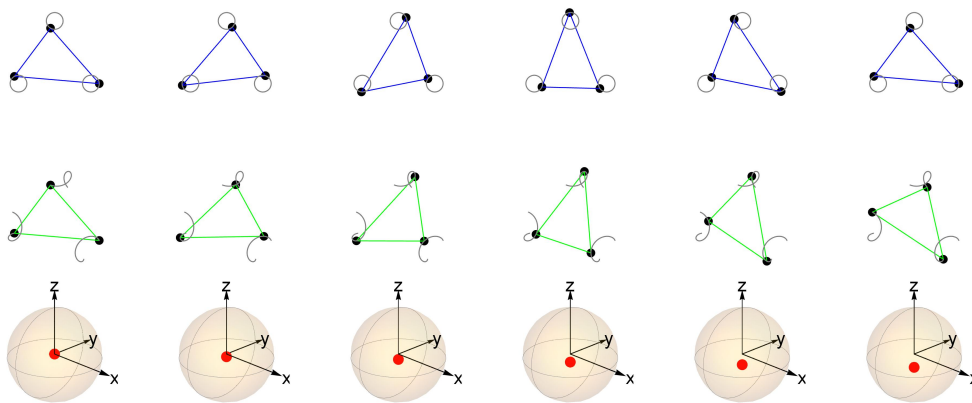

Figure 3: Sequence of the orientation change produced by a cyclic deformation in shape space for the three-body problem. The top and middle rows are the snapshots of the deformation in the body (blue) and space (green) frames at times $t = 0, 2\pi/5, \ldots, 2\pi$. The circle and cycloid-like lines in the snapshots are the trajectories of the particles in the body and space frame, respectively. Each particle rotates counterclockwise around a certain point, and to preserve the vanishing total angular momentum, the whole system must rotate clockwise, as it is observed in the space frame. The bottom row is the rotation in $SO(3)$ in the axis-angle representation. The red dot is the rotation between the body and space frame.

As we mentioned before, the equation (11) gives, in general, a non-trivial connection when $L = 0$, and therefore the system may obtain an orientation change induced by shape deformations. In the three-body problem, the connection may produce anholonomy by its non zero Coriolis tensor,

$$B_{\mu\nu} = \frac{1}{2q_3^2}\varepsilon_{\mu\nu\alpha}q^{\alpha}_{\hat{z}} \tag{25}$$

For instance, the path trajectory in the shape space

$$q_1 = \frac{1}{2} sin(\omega t), \quad q_2 = \frac{1}{2} cos(\omega t), \quad q_3 = 1, \tag{26}$$

induces a re-orientation of the system monitored in Fig. 3. In the last row, we plot the orientation (red dot) of the system with respect to the space frame in the axis-angle representation of *SO(3)*. In Ref. (Chryssomalakos et al., 2015), the authors use coherent states in the shape space to reproduce this evolution in the quantum version of the system.

IV | QUANTUM CASE

In the quantum regime, the system lacks a well-defined shape and orientation. Now, the system is in a superposition of states, each corresponding to a definite shape and orientation. The general quantum state will be described by a wavefunction $\Psi(\mathsf{R}, q^\mu)$ con C which codifies the probability to find the state in the configuration (R, q^μ) for each point of C . The values of the shape and angular momentum are now expectation values, $\langle\Psi|q^\mu|\Psi\rangle$ and $\langle\Psi|L_s|\Psi\rangle$. Additional to this, the condition $\langle L_s\rangle = 0$ does not imply that $\langle L\rangle$ vanishes because the rotation between the body and space frame $\mathsf{R}(q^\mu)$ is a shape dependent operator. The quantized Hamiltonian has the same expression as (14) with the same ordering and an additional potential $V_2(q)$ (Littlejohn & Reinsch, 1997) given by

$$V_2(q) = \frac{\hbar^2}{2} D^{-1/4} \frac{\partial}{\partial q^\mu} \left(g^{\mu\nu} \frac{\partial D^{1/4}}{\partial q^\nu} \right), \tag{27}$$

with $D = (\det \mathsf{M})(\det g_{\mu\nu})$. H commutes with $\mathbf{L}^2$ and $\mathbf{L}_{sz}$ in the three-body case, so its eigenfunctions $\Psi(\mathsf{R}, q)$ are labeled by the quantum numbers E, l, m, respectively, which we denote by $\Psi_{Elk}(\mathsf{R}, q)$. The wavefunction over a section Σ of the configuration space has the form

$$\chi_k^{El}(q) = \frac{1}{\sqrt{2l+1}} \Psi_{Elk}(\mathbb{1}, q), \tag{28}$$

where k is the quantum number of the angular momentum in the body frame L_z and $\mathbb{1}$ is the identity element of $SO(3)$. By angular momentum theory, the complete wavefunction can be expressed with $\chi_k^{El}(q)$,

$$\Psi_{Elm}(\mathsf{R}, q) = \sum_{k=-l}^{l} \chi_k^{El}(q) D^l_{mk}(\mathsf{R}) *, \tag{29}$$

where $D^l_{mk}(\mathsf{R})$ are the Wigner D functions corresponding to the irreducible $(2l+1)\cdot(2l+1)$ matricial representation (irrep) of $SO(3)$. The functions $\mathbf{A}_\mu$, M, $g_{\mu\nu}$ and V, are now complicated shape operators. To handle them, we will consider some approximations.

1 | Approximations

For the aim of the paper, it is not necessary to solve the Hamiltonian in the general case. We assume that: (i) the wavefunction is factorizable $\Psi(\mathsf{R}, q) = \Phi(\mathsf{R})\psi(q)$, and (ii) the time evolution is a Born-Oppenheimer like approximation, where the evolution of the shape wavefunction is not affected by the orientation wavefunction. The first assumption will give us a clear division between the shape and orientation wavefunctions for initial values of time. The evolution of the system will vanish the

factorization of the wavefunction gradually. The second assumption is justified by the fact that the vibrational states require more energy to get excited than the rotational ones in molecular systems. The last assumption appears in many studies without mention, for instance, in the calculation of the so-called rotational constants (Yamanouchi, 2012) which are related to the inertia moments of a system with an implicit supposed fixed shape. Applying these approximations, the Hamiltonian of the shape wavefunction $\psi(q)$ is

$$H_s = p_\mu g^{\mu\nu} p_\nu + V(q) + V_2(q). \tag{30}$$

The last Hamiltonian is still a formidable problem to solve in most of the cases, which it is not our purpose. Then, instead of that, we will choose a specific $\psi(q,t)$ y physical considerations. The Hamiltonian of the orientation wavefunction is

$$2H_O = \mathbf{L}\cdot \mathsf{M}^{-1}\cdot\mathbf{L} + g^{\mu\nu}(\mathbf{A}_\mu\cdot\mathbf{L})(\mathbf{A}_\nu\cdot\mathbf{L}) - p_\mu g^{\mu\nu}(\mathbf{A}_\nu\cdot\mathbf{L}) - (\mathbf{A}_\mu\cdot\mathbf{L})g^{\mu\nu}p_\nu, \tag{31}$$

where the shape operators are now expectation values of $y(q;t)$. For instance, the factors in the second term of the r.h.s.of equation (31) are now the time functions $\langle\psi(q,t)|g^{\mu\nu}A_{\mu i}A_{\nu j}|\psi(q,t)\rangle$.

2 | Orientation wavefunction

We want an appropriate orientation wavefunction with $\langle L\rangle = \langle L_s\rangle = 0$, and with a localized orientation to follow its changes. Considering that the body and space frames coincide in the localized orientation, the maximum of the orientation wavefunction will be in the origin of the angle-axis representation of $SO(3)$. The orientation wavefunction must not depend on the rotation axis (θ,ϕ) to avoid a preference direction. We call the former kind of orientation wavefunctions *isotropic* we call the former kind of orientation wavefunctions *isotropic*. In the literature, they are called *class functions*.

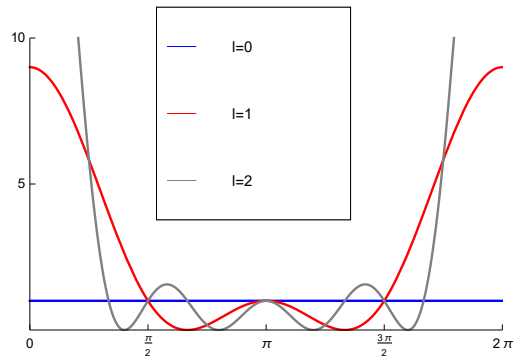

Figure 4: $|\chi^l(\eta)|^2$ for $l = 0,1,2$.

For a spin representation l, a general wavefunction on *SO(3)* $\Phi(\eta;\theta,\phi)$ is given by

$$\Phi(\eta;\theta,\phi) = \sum_{mk} c_{mk} D^l_{mk}(\eta;\theta,\phi). \tag{32}$$

$\Phi(\mathsf{R})$ will not depend of the rotation axis if it is invariant under rotations,

$$\Phi(\mathsf{R}) = \Phi(\mathsf{URU}^{-1}), \quad \forall U \in SO(3). \tag{33}$$

Well-known functions with this property are the characters $\chi^l(\mathsf{R})$ of the irrep of the *SO(3)* group (Varshalovich, Moskalev, & Khersonskii, 1988),

$$\chi^l(\eta) = \chi^l(\mathsf{R}) = \sum_{m=-l}^{m} D^l_{mm}(\mathsf{R}). \tag{34}$$

In fact, they are the only functions independent of the rotation axis. To prove the last statement, we expand (omitting the upper index l) eq. (33)

$$\sum_{m,k} c_{mk} D_{mk}(\mathsf{R}) = \sum_{m,k,m',m''} c_{mk} D_{mm_0}(\mathsf{U}) D_{k_0k}(\mathsf{U}^{-1}), \tag{35}$$

and express an equation between the c_{mk} coefficients,

$$c_{m_0k_0} = \sum_{m,k} c_{mk} D_{mm_0}(\mathsf{U}) D_{k_0k}(\mathsf{U}^{-1}), \tag{36}$$

The only way to satisfy the last equation is with the condition $c_{mk} = \delta_{mk} c$ and the relation

$$\sum_{m''} D_{mm''}(U) D_{m''m'}(U^{-1}) = \delta_{mm'}. \tag{37}$$

An expression of the characters $\chi^l(\eta)$ is the following (Varshalovich et al., 1988)

$$\chi^l(\eta) = \frac{sin\,[2l+1]\,\frac{\eta}{2}}{sin\,\frac{\eta}{2}}. \tag{38}$$

The last expression tells us that the maximum of $\chi^l(\eta)$ are in $\eta = 0$ and therefore, the isotropic wavefunctions are the linear combination of $\chi^l(\eta)$. The Fig. 4 shows the probability density of $|\chi^l(\eta)|^2$ for $l = 0, 1, 2$. The state is more localized when you increase the value of l. A rotation $\eta > \pi$ along the vector $\hat{\mathbf{n}}$ is equivalent to a rotation of $\eta - \pi$ in the antipodal direction.

V | THREE- BODY QUANTUM SYSTEM

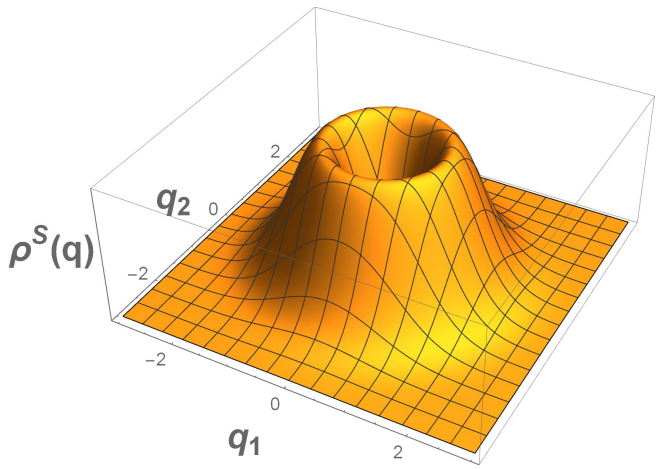

Figure 5: ρ^s of the shape wavefunction (42).

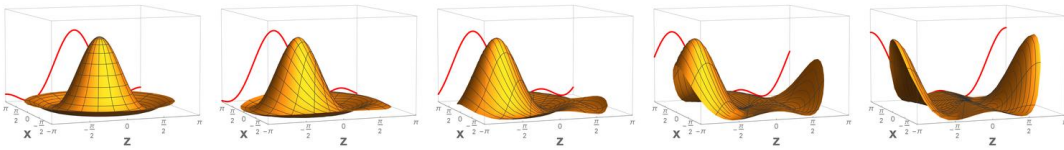

Figure 6: Evolution of the orientation change of the quantum system (46). We consider only the evolution given by the interaction Hamiltonian H_I. The snapshots contain plots of the reduced probability density $\rho_t^O(\mathsf{R})$, restricted to the xz-plane of $SO(3)$ in the angle-axis representation for $t = \pi n/4$, $n = 0,1,\ldots,4$ (elsewhere in $SO(3)$, $\rho_t^O(\mathsf{R})$ is obtained by rotation around the $\hat{z}$ axis). The red curve is the silhouette of $\rho_t^O(\mathsf{R})$ in the $\hat{z}$ axis of $SO(3)$. The evolution is given by a consecutive rigid rotation, ending with a rotation by π around the $\hat{z}$.

We use the three-body system presented in section III, with the shape coordinates (17) and the northregular gauge (18). The equations (20) are substituted in (31), and the Hamiltonian takes the form

$$2H_O = \left(\frac{q+q_1}{q_3^2}\right)L_x^2 + \left(\frac{q-q_1}{q_3^2}\right)L_y^2 + \left(\frac{1}{q+q_3}\right)L_z^2 + \left(\frac{q_2}{q_3^2}\right)(L_xL_y + L_yL_x) + \frac{2L_z}{q+q_3}(q_2p_1 - q_1p_2). \tag{39}$$

To make the results as analytic as possible we consider $\langle q_3\rangle$ constant over time and such that $|\langle q_3\rangle| \gg |\langle q_1(t)\rangle|, |\langle q_2(t)\rangle|$. With this approximation, $\langle q\rangle \approx \langle q_3\rangle \equiv a$. The last approximation assumes that the mean distance of the particles with respect to the center of mass is bigger than the periodical displacements produced by q_1 y q_2. Now, for a fixed value of l, the orientational Hamiltonian has a constant term which can be omitted $H_O' = 2a^2H_O - \frac{a}{2}l(l+1)$ and is divided in two parts

$$\begin{aligned} H_O' &= H_L + H_I \\ H_L &= \left(\frac{a}{2}+q_1\right)L_x^2 + \left(\frac{a}{2}-q_1\right)L_y^2 + q_2(L_xL_y + L_yL_x) \\ H_I &= aL_z(q_2p_1 - q_1p_2) \end{aligned} \tag{40}$$

1 | Rotations induced by a static shape

We consider $m = a = \hbar = 1$. To be able to monitor visually the system's evolution, we start from the probability density $\rho_t(\mathsf{R},q) = |\Phi(\mathsf{R},q)|^2$ and compute reduced densities

$$\rho_t^s(q) = \int \rho_t d\mathsf{R}, \quad \rho_I^O(\mathsf{R}) = \int \rho_t \sqrt{g} d^{3n-6}q, \tag{41}$$

in shape space and *SO(3)*, respectively. We consider the shape wavefunction given by the eigenstates of the harmonic oscillator in the normal modes $q_1, q_2, |n_1,n_2\rangle, |\psi\rangle = \frac{1}{\sqrt{2}}(|1,0\rangle + i|0,1\rangle)$, with wavefunction

$$\psi(q) = \frac{1}{2\pi}e^{-\frac{(q_1^2+q_1^2)}{2}}[H_1(q_1)H_0(q_2) + iH_0(q_1)H_1(q_2)] = \frac{1}{\sqrt{\pi}}e^{-\frac{(q_1^2+q_1^2)}{2}}(q_1+iq_2) \tag{42}$$

where $H_n(x)$ are the Hermite polynomials and $\omega = 1$. The plot of $\rho_t^S(q)$ is in Fig. 5.$\rho_t^S(q)$ doesn't change on time and their most probable shape configurations are on a circle in the $q_1 - q_2$ plane around the configuration $(q_1, q_2, q_3) = (0, 0, a)$. Even when the quantum shape of the system doesn't change, H_1 is not zero,

$$\langle q_1 \rangle = \langle q_2 \rangle = 0 \quad , \quad \langle q_1 p_2 - q_2 p_1 \rangle = 1 \tag{43}$$

To deduce the origin of the non zero expectation value, we decompose $\psi(q) = \sqrt{\rho(q)} e^{iS(q)}$ and calculate the real part of the expression

$$\mathrm{Re}(\psi^*(q_1 p_2 - q_2 p_1)\psi) = \rho(q_1 \partial_{q_2} S - q_2 \partial_{q_1} S) \tag{44}$$

The imaginary part does not contribute to the expectation value. The wavefunction (42) has

$$\sqrt{\rho} = \sqrt{\frac{q_1^2 + q_2^2}{\pi}} \exp\left(-\frac{q_1^2 + q_1^2}{2}\right) \quad , \quad \cos S = \frac{q_1}{\sqrt{q_1^2 + q_2^2}} \tag{45}$$

The operator (44) measures the rotational of the function S, which in this case it does have. In this way, the interaction Hamiltonian H_1, which relates the dynamics between the shape and orientation degrees of freedom gives a rotation to the system, even when the shape reduced density $\rho_t^S(q)$ does not change on time. The system has a probability current surrounding the $\hat{z}$ axis. This flux adjudge an angular momentum which is invisible in $\rho_t^S(q)$, and by H_1 imposes a rotation in the system $U_1(t) = e^{itL_z}$. We show in Fig. (6) the evolution of $\rho_t^O(R)$ induced by the interaction Hamiltonian H_1 of the state

$$\Psi(\mathsf{R}, q) = \chi^l(\mathsf{R})\psi(q), \tag{46}$$

with $l = 1$ and shape wavefunction (42). The quantum body rotates rigidly around the $\hat{z}$-axis produced by its static *quantum shape*.

2 | Rotation induced by H_L

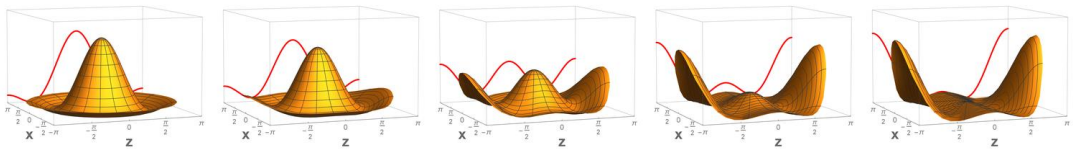

Figure 7: Sequence of the $\rho_t^O(\mathsf{R}) = |\chi^1(\mathsf{R})|^2$ evolution produced by H_L with shape wavefunction (42) for $t = 2\pi n/4$, $n = 0, 1, \ldots, 4$. $\rho_t^O(\mathsf{R})$ at times $t = 0, 2\pi$ differs by a displacement of π along the $\hat{z}$ axis, which means that the system gets a rotation by π around the $\hat{z}$-axis.

Now, we study the rotational effects produced by the Hamiltonian term H_L in the isotropic wavefunctions. We assume H_L given by the shape wavefunction (42),

$$H_L = \frac{1}{2}(L_x^2 + L_y^2) = \frac{1}{2}(\mathbf{L}^2 - L_z^2) \tag{47}$$

H_L is equivalent (plus a factor) of the rigid rotor Hamiltonian of a three-body system in an equilateral triangle configuration with equal masses. In the classical case, a system with vanishing angular momentum does not obtain an evolution by this term. However, in the quantum case is different, $\chi^l(\mathsf{R})$ obtains a non-trivial evolution. We plot in Fig. (7) the $U_L = e^{-iH_L t}$ evolution of $\rho_t^O(\mathsf{R}) = |\chi^l(\mathsf{R})|^2$ with $l = 1$, at times $t = 2\pi n/4,\ n = 0, 1, ..., 4$. The central peak of the orientation wavefunction shrinks and the small peak in π increases over time. At $t = 2\pi$, the system recovers its localized aspect seen at $t = 0$ displaced by π along the $\hat{z}$ axis. It means that H_L by itself may produced net rotations independent of the induced rotation by the shape wavefunction and which is not produced, at least explicitly, with some sort of angular momentum. A similar evolution is observed for any isotropic wavefunction. To prove this statement, we compare two evolutions of $\chi^l(\eta)$ produced by $U_L(t = 2\pi) = e^{-i\pi(\mathbf{L}^2 - L_z^2)}$ and $U_1(t = \pi) = e^{i\pi L_z}$, respectively,

$$\begin{aligned} U_L(t = 2\pi)\chi^l(\eta) &= N e^{-i\pi l(l+1)} \left(\sum_m e^{i\pi m^2} D_{mm} \right) \\ &= N \left(\sum_m (-1)^{-m} D_{mm} \right) \\ &= U_L(t = \pi)\chi^l(\eta), \end{aligned} \tag{48}$$

where $U_L(t = \pi)$ is a rigid rotation around the $\hat{z}$-axis. As we observe, this result is independent of l and then, any linear combination of $\chi^l(\eta)$ (isotropic wavefunction) will have the same behavior.

VI | CONCLUSIONS

We show a rotating quantum system (46) with $\langle \mathbf{L} \rangle = \langle \mathbf{L}_s \rangle = 0$ and rigid *quantum shape*, observed in the reduced probability density $\rho_t^S(q)$ (Fig.5). The induced rotation comes from the probability current, which could exist even without a real changing of the *shape system*. It could be thought as a car tire who rotates unde its axis of symmetry. The rubber density is constant over the time but it still has a non zero angular momentum. In an analogous case than the classic problem, the shape wavefunction has an *internal* angular momentum (43) which induces a rotation to the whole system to keep the total angular momentum zero. This example shows a system which it doesn't change its internal (shape) configuration and then its internal physical properties. For instance, if we consider this system as a model of a molecular or nuclear system, or a nano-system, the magnitude of the expectation values of the electric and magnetic multipolar moments doesn't change on time, and even without angular momentum, the direction of these physical quantities of the system could stay rotating. The same phenomenon is produced in n-body systems with $n > 3$, with aditional touches emerging since the four body system because now the system can be non-planar.

Another result presented in the paper is the characterization of the isotropic orientation wavefunctions, defined as the wavefunctions in *SO(3)* which doesn't depend on the rotation axis. The constituents of the isotropic wavefunctions are the characters $\chi^l(\mathsf{R})$ of the irrep of *SO(3)* which are states localized in the origin and represent systems with a localized orientation and $\langle \mathbf{L} \rangle = \langle \mathbf{L}_s \rangle = 0$. Any wavefunction $\Phi(R)$ with a localized orientation can be written as a linear combination of the characters $\chi^l(\mathsf{R})$, rotated by some R'. We observe that the evolution of the isotropic wavefunctions induced by a rigid rotor-like Hamiltonian, for instance, H_L in eq. (V), could induce a rotation by π around some axis. In our three-body system with an equilateral triangle shape, it means that the equilateral triangle, initially in a particular orientation, after some time, it will be re-oriented by a rotation of π around the $\hat{z}$-axis. This result persists for any system with localized orientation wavefunction and shape with two-degenerated

principal moments of inertia. In future work, the evolution of isotropic wavefunctions for more general Hamiltonians will be studied with more detail.

REFERENCES

Chryssomalakos, C., Hernández-Coronado, H., & Serrano-Ensástiga, E. (2015). Do free-falling quantum cats land on their feet? *J. Phys. A.*, *48*, 295301.

Frolich, C. (1979). Do springboards divers violate angular momentum conservation? *Am. J. Phys.*, *47*, 583–592.

Guichardet, A. (1984). On rotation and vibration motions of molecules. *Ann. Inst. H. Poincaré, Phys. Theor.*, *40/3*, 329–342.

Iwai, T. (1987). A gauge theory for the quantum planar three-body problem. *J. Math. Phys.*, *28*.

Kane, T. R., & Scher, M. P. (1969). A dynamical explanation of the falling cat phenomenon. *Int. J. Solids Struct.*, *5*, 663–670.

Kottas, G. S., Clarke, L. I., Horinek, D., & Michl, J. (2005). Artificial molecular rotors. *Chem. Rev.*, *105*, 1281–1376.

Littlejohn, R. G., Mitchell, K. A., Reinsch, M., Aquilanti, V., & Cavalli, S. (1998a). Body frames and frame singularities for three-atom systems. *Phys. Rev. A*, *58/5*, 3705–3717.

Littlejohn, R. G., Mitchell, K. A., Reinsch, M., Aquilanti, V., & Cavalli, S. (1998b). Internal spaces, kinematic rotations, and body frames for four-atom systems. *Phys. Rev. A*, *58/5*, 3718–3738.

Littlejohn, R. G., & Reinsch, M. (1997). Gauge fields in the separation of rotations and internal motions in the *n*-body problem. *Rev. Mod. Phys.*, *69/1*, 213–275.

Mitchell, K. A., & Littlejohn, R. G. (1999). The rovibrational kinetic energy for complexes of rigid molecules. *Mol. Phys*, *96*(9), 1305-1315.

Mitchell, K. A., & Littlejohn, R. G. (2000). Boundary conditions on internal three-body wave functions. *Phys.Rev. A*, *61*, 042502.

Montgomery, R. (1993). Gauge theory of the falling cat. *Fields Inst. Commun.*, *1*, 193–218.

Nakahara, M. (1990). *Geometry, Topology and Physics*. Institute of Physics Publishing.

Ohmann, R. (2015). Supramolecular rotor and translator at work: On-surface movement of single atoms. *ACS Nano*, *9*(8), 8394–8400.

Ovchinnikov, A. A., Erikhman, N. S., & Pronin, K. A. (2001). *Vibrational-rotational excitations in nonlinear molecular systems*. Springer Science.

Perera, U. G. E. (2013). Controlled clockwise and anticlockwise rotational switching of a molecular motor. *Nat. Nanotechnol.*, *8*, 46-51.

Shapere, A., & Wilczek, F. (1989). Gauge kinematics of deformable bodies. *Am. J. Phys.*, *57*, 514–518.

Tachibana, A., & Iwai, T. (1986). Complete molecular hamiltonian based on the born-oppenheimer adiabatic approximation. *Phys. Rev. A*, *33/4*, 2262–2269.

Tennyson, J., & Sutcliffe, B. T. (1982). The ab initio calculation of the vibrational-rotational spectrum of triatomic systems in the close coupling approach, with kcn and $h_2$ne as examples. *J. Chem. Phys.*, *77*, 4061.

Varshalovich, D. A., Moskalev, A. N. ., & Khersonskii, V. K. . (1988). *Quantum Theory of Angular Momentum*. World Scientific.

Yamanouchi, K. (2012). *Quantum mechanics of molecular structures*. Springer.