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Eckart frame Hamiltonians in the three-body problem

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Abstract The Eckart frame is used to separate out the collective rotations in the quantum three-body problem. Explicit expressions for the corresponding rotational and vibro-rotational (i.e. Coriolis) Hamiltonians are derived. Special attention is paid to the situation when two principal moments of inertia are equal in the equilibrium configuration.

Keywords Vibrations and rotations · Coriolis couplings · Eckart frame · Molecular Hamiltonians

1 Introduction

The theoretical study of various properties of molecules and atomic nuclei requires the separation of their motion into the vibrational and rotational parts. Such a separation can be achieved by introducing the rotating reference frame (the body-frame, BF) whose axes are defined by the orientation of the whole system in space. As a result, the motion of particles with respect to BF can be considered as "vibration" while the motion of BF itself can be understood as the overall "rotation". At this stage the question occurs as to how to choose BF in an optimal way.[1] An optimal BF would be that in which the couplings between the vibrations and the overall rotation are minimal.

C. Eckart [2] introduced BF which minimizes the vibro-rotational (or, Coriolis) couplings in case when particles of the system perform small vibrations close to some equilibrium configuration. The Eckart BF is that in which the following relation is fulfilled

[1] Since the choice of BF is not unique, its definition can be considered as the gauge convention [1].

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$$m_1 [\mathbf{R}_1 \times \mathbf{R}_1^{(eq)}] + m_2 [\mathbf{R}_2 \times \mathbf{R}_2^{(eq)}] + m_3 [\mathbf{R}_3 \times \mathbf{R}_3^{(eq)}] = 0, \tag{1}$$

where $\mathbf{R}_i^{(eq)}$ is the equilibrium value of the position vector $\mathbf{R}_i$ of the particle with the mass m_i. The above equation is usually called "the second Eckart condition" [2,3]. (The first Eckart condition is the requirement of the origin of BF to be at c.m. of the system.)

The Eckart BF has been studied for a long time [4–21]. The reason is that the vibro-rotational decomposition of the Hamiltonian corresponding to Eckart BF has some attractive features. One of which is that the Coriolis Hamiltonian in the Eckart frame is small for small-amplitude vibrations. Despite the broad literature on the topic some problems still remain. Namely, existing results related to the three-body problem are rather cumbersome. They also do not exhibit simple behavior in the rigid-body limit when vibrations tend to zero. In this limit the Coriolis (i.e. vibro-rotational) part of Eckart frame Hamiltonian vanishes and the rotational part of the kinetic energy becomes that of a rigid body.

The goal of this article is to present the vibro-rotational Hamiltonians to the Eckart frame in most simple and compact form such that their rigid-body limit would be obvious. The consideration is based on the general formalism developed in [22,23].

The procedure of the separation of rotations and vibrations consists in the transformation of the total Hamiltonian into three parts

$$H = H_0 + H_{cor} + H_{rot}, \tag{2}$$

where H_0 is the vibrational Hamiltonian, H_{rot} is the rotational Hamiltonian which is quadratic in the components of the total angular momentum $\mathbf{L}$ given in BF, and H_{cor} is the vibro-rotational (Coriolis) Hamiltonian which is linear both in components of $\mathbf{L}$ and the vibrational linear momenta.

2 The kinetic energy and Eckart condition in terms of Jacobi vectors

Assuming that the center of mass of the system is at the origin of the coordinate frame the Schrödinger equation for the system of three particles can be written as [1,24]

$$\left(-\frac{1}{2\mu_1} \frac{\partial^2}{\partial \mathbf{r}_1^2} - \frac{1}{2\mu_2} \frac{\partial^2}{\partial \mathbf{r}_2^2} + U - E \right) \Psi(\mathbf{r}_1, \mathbf{r}_2) = 0. \tag{3}$$

where U is the potential energy operator which depends on three internal variables; $\mathbf{r}_1$ and $\mathbf{r}_2$ are Jacobi vectors (see Fig. 1) and the reduced masses μ_1, μ_2 are defined by

$$\frac{1}{\mu_1} = \frac{1}{m_2} + \frac{1}{m_3}, \quad \frac{1}{\mu_2} = \frac{1}{m_1} + \frac{1}{m_2 + m_3}. \tag{4}$$

The second Eckart condition in terms of Jacobi vectors reads

$$\mu_1 [\boldsymbol{\rho}_1 \times \mathbf{r}_1] + \mu_2 [\boldsymbol{\rho}_2 \times \mathbf{r}_2] = 0. \tag{5}$$

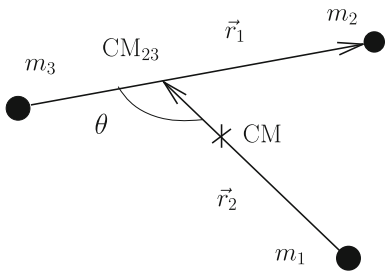

Fig. 1 Jacobi vectors for the three-body system. CM_{23} is the CM of the particles m_2 and m_3

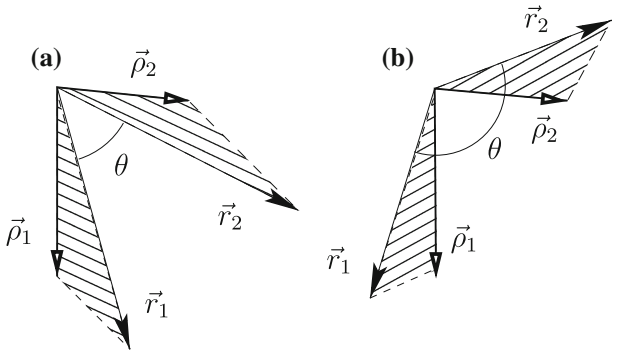

Fig. 2 The geometrical meaning of the Eckart condition. **a** the mutual angle between Jacobi vectors is $\theta < \pi/2$, **b** the mutual angle is $\theta > \pi/2$. On each figure the areas of the *dashed triangles* are equal

It is convenient to introduce the so-called "mass-scaled" Jacobi vectors by replacing $\mathbf{r}_1 \to \mathbf{r}_1/\sqrt{\mu_1}, \mathbf{r}_2 \to \mathbf{r}_2/\sqrt{\mu_2}$ (and analogously for $\boldsymbol{\rho}_{1,2}$).

In terms of mass-scaled Jacobi vectors the Schrödinger equation becomes

$$\left(-\frac{1}{2}(\Delta_1^2 + \Delta_2^2) + U - E\right)\Psi(\mathbf{r}_1, \mathbf{r}_2) = 0, \tag{6}$$

and the second Eckart condition reads

$$[\boldsymbol{\rho}_1 \times \mathbf{r}_1] + [\boldsymbol{\rho}_2 \times \mathbf{r}_2] = 0. \tag{7}$$

This condition has simple geometrical meaning. Namely, according to (7), the areas of two triangles build on pairs of vectors $\boldsymbol{\rho}_1, \mathbf{r}_1$ and $\boldsymbol{\rho}_2, \mathbf{r}_2$ must be equal, see Fig. 2.

The equilibrium vectors $\boldsymbol{\rho}_{1,2}$ are not moving in BF and they define the basis vectors of BF. Let us assume that BF basis vectors are directed along the main axes of the inertia tensor in the equilibrium configuration. The decomposition of the vectors $\boldsymbol{\rho}_{1,2}$ over the BF basis vectors $\mathbf{e}_1, \mathbf{e}_2$ can be written as

$$\begin{aligned} \boldsymbol{\rho}_1 &= x_1\,\mathbf{e}_1 + y_1\,\mathbf{e}_2, \\ \boldsymbol{\rho}_2 &= x_2\,\mathbf{e}_1 + y_2\,\mathbf{e}_2, \end{aligned} \tag{8}$$

where (x_k, y_k) are Cartesian components of $\boldsymbol{\rho}_k$ $(n = 1, 2)$ in BF. Now let us introduce Eckart vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ by

$$\begin{aligned} \mathbf{f}_1 &= x_1\,\mathbf{r}_1 + x_2\,\mathbf{r}_2, \\ \mathbf{f}_2 &= y_1\,\mathbf{r}_1 + y_2\,\mathbf{r}_2. \end{aligned} \tag{9}$$

Inserting (8) into (7) one arrives at the following representation of the Eckart condition

$$[\mathbf{e}_1 \times \mathbf{f}_1] + [\mathbf{e}_2 \times \mathbf{f}_2] = 0. \tag{10}$$

The solution of this equation has been obtained in [23] and it reads

$$\begin{aligned} \mathbf{e}_1 &= \frac{1}{\mathcal{F}}\left(\mathbf{f}_1 + \frac{[\mathbf{f}_2 \times [\mathbf{f}_1 \times \mathbf{f}_2]]}{|\mathbf{f}_1 \times \mathbf{f}_2|}\right), \\ \mathbf{e}_2 &= \frac{1}{\mathcal{F}}\left(\mathbf{f}_2 - \frac{[\mathbf{f}_1 \times [\mathbf{f}_1 \times \mathbf{f}_2]]}{|\mathbf{f}_1 \times \mathbf{f}_2|}\right), \end{aligned} \tag{11}$$

where the Eckart parameter $\mathcal{F}$ is defined by

$$\mathcal{F} = \sqrt{f_1^2 + f_2^2 + 2\,|\mathbf{f}_1 \times \mathbf{f}_2|}. \tag{12}$$

The orthogonality and normalization of vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ as well as their compliance with the Eckart condition (10) can be easily proved by straightforward computations.

The Eckart parameter $\mathcal{F}$ can also be written as [23],

$$\mathcal{F} = (\mathbf{e}_1 \cdot \mathbf{f}_1) + (\mathbf{e}_2 \cdot \mathbf{f}_2). \tag{13}$$

This equation clarifies the meaning of the Eckart parameter. As is seen, $\mathcal{F}$ is the sum of projections of Eckart vectors on the corresponding basis vectors of Eckart BF.

3 Eckart internal variables

We choose the set of internal variables to be the lengths of the Eckart vectors f_1, f_2 and cosine of their mutual angle $\tau = \cos\phi = (\mathbf{f}_1 \cdot \mathbf{f}_2)/(f_1 f_2)$. In order of derive the expression for the kinetic energy operator we note the connection between the gradient operators in terms of Jacobi and Eckart vectors,

$$\frac{\partial}{\partial \mathbf{r}_\alpha} = x_\alpha \frac{\partial}{\partial \mathbf{f}_1} + y_\alpha \frac{\partial}{\partial \mathbf{f}_2}, \quad \alpha = 1, 2. \tag{14}$$

From this equation one can derive the expression for the kinetic energy,

$$\nabla_1^2 + \nabla_2^2 = I_2\,\tilde{\nabla}_1^2 + I_1\,\tilde{\nabla}_2^2, \tag{15}$$

where $\tilde{\nabla}_{1,2}$ is the gradient operator with respect to $\mathbf{f}_{1,2}$ and $I_2(I_1)$ is the equilibrium moment of inertia with respect to $y-(x-)$ axis (see Appendix B),

$$I_1 = y_1^2 + y_2^2, \quad I_2 = x_1^2 + x_2^2. \tag{16}$$

When deriving (15) we have used the fact that the axes of BF are directed along the principal axes of the equilibrium inertia tensor, so that

$$x_1 y_1 + x_2 y_2 = 0. \tag{17}$$

The connection of the Eckart internal variables with the Jacobi-bond variables follows from the definition (9) of vectors $\mathbf{f}_{1,2}$ and is given in Appendix A.

The above Eq. (15) allows one to derive the expression for the vibrational kinetic energy in terms of variables f_1, f_2, τ. Omitting details of some routine computations which are analogous to those presented in [22] the final result reads

$$H_0 = -\sum_{i=1}^{2} \frac{I_i}{2f_i^2} \frac{\partial}{\partial f_i} f_i^2 \frac{\partial}{\partial f_i} - \frac{1}{2}\left(\frac{I_1}{f_1^2} + \frac{I_2}{f_2^2}\right) \frac{\partial}{\partial \tau}(1-\tau^2)\frac{\partial}{\partial \tau} + U(f_1, f_2, \tau), \tag{18}$$

where U denotes the potential energy which depends only on the internal variables.

4 The Coriolis Hamiltonian

In [22,23] the general expression for the Coriolis Hamiltonian has been found which is

$$H_{cor} = i \sum_{k=1}^{3} L_k \left(\sum_{\gamma=1}^{3} C_{\gamma k}(\xi) \frac{\partial}{\partial \xi_\gamma} + B_k(\xi) \right). \tag{19}$$

Here, L_k denotes the projection of the total angular momentum operator on the k-th axis of BF ($k = 1, 2, 3$) and the parameters $C_{\gamma k}$ and B_k are determined by the differential properties of BF basis vectors. For the Eckart BF these parameters were calculated in [23].

In the three-body problem among parameters B_k only B_3 is non-zero [23],

$$B_3 = \frac{I_2 - I_1}{\mathcal{F}^2} \frac{(\mathbf{f}_1 \cdot \mathbf{f}_2)}{|\mathbf{f}_1 \times \mathbf{f}_2|} = (I_2 - I_1) \frac{\cot \phi}{\mathcal{F}^2}, \tag{20}$$

where the Eckart parameter $\mathcal{F}$ is defined by (12).

The parameters $C_{\gamma k}$ depend on the choice of the internal variables. The expression for $C_{\gamma k}$ is given in [23],

$$C_{\gamma k} = -\sum_{ijq}(\mathbf{U}^{-1})_{kq}\,\epsilon_{ijq}\,\sum_{\alpha}\eta_{\alpha i}\,(\mathbf{e}_j\cdot\nabla_\alpha)\,\xi_\gamma = -\sum_{q}(\mathbf{U}^{-1})_{kq}\sum_{\alpha=1}^{2}(\mathbf{e}_q\cdot[\boldsymbol{\rho}_\alpha\times\nabla_\alpha])\,\xi_\gamma \tag{21}$$

Here, ϵ_{ijq} is the unit totally antisymmetric tensor, $\mathbf{U}^{-1}$ is a 3×3-matrix whose elements depend on ξ. In the three-body problem explicit form of $\mathbf{U}^{-1}$ can be obtained using results of [23],

$$\mathbf{U}^{-1} = \frac{1}{\mathcal{F}\,|\mathbf{f}_1\times\mathbf{f}_2|}\begin{pmatrix} |\mathbf{f}_1\times\mathbf{f}_2| + f_1^2 & (\mathbf{f}_1\cdot\mathbf{f}_2) & 0 \\ (\mathbf{f}_1\cdot\mathbf{f}_2) & |\mathbf{f}_1\times\mathbf{f}_2| + f_2^2 & 0 \\ 0 & 0 & |\mathbf{f}_1\times\mathbf{f}_2| \end{pmatrix}. \tag{22}$$

Noting the definition (9) of Eckart vectors, expression (14) for the gradient operators ∇_α and the property (17) one can prove that the equation

$$\sum_{\alpha=1}^{2}[\boldsymbol{\rho}_\alpha\times\nabla_\alpha] = I_2\,[\mathbf{e}_1\times\tilde{\nabla}_1] + I_1\,[\mathbf{e}_2\times\tilde{\nabla}_2] \tag{23}$$

is valid. The action of the operators $\tilde{\nabla}$ on the internal variables ξ gives a vector lying in the xy-plane of BF. This fact, together with (22), leads to the conclusion that among coefficients $C_{\gamma k}$ only $C_{\gamma 3}$ is non-zero. It is

$$C_{\gamma 3} = -\frac{1}{\mathcal{F}}\left(I_2(\mathbf{e}_2\cdot\tilde{\nabla}_1) - I_1(\mathbf{e}_1\cdot\tilde{\nabla}_2)\right)\xi_\gamma. \tag{24}$$

This equation is the main result of the present section.

The set of C-coefficients corresponding to Eckart internal variables $\xi = (f_1, f_2, \cos\phi)$ defined in Sect. 3 can easily be obtained using (24). The result reads

$$\begin{aligned} C_{13} &= -\frac{I_2}{\mathcal{F}\,f_1}(\mathbf{e}_1\cdot\mathbf{f}_1) = -I_2\frac{(\mathbf{f}_1\cdot\mathbf{f}_2)}{\mathcal{F}^2 f_1}, \\ C_{23} &= -\frac{-I_1}{\mathcal{F}\,f_2}(\mathbf{e}_1\cdot\mathbf{f}_2) = I_1\frac{(\mathbf{f}_1\cdot\mathbf{f}_2)}{\mathcal{F}^2 f_2}, \\ C_{33} &= -\frac{\sin\phi}{\mathcal{F}^2}\left(I_2 - I_1 + \sin\phi\left(I_2\frac{f_2}{f_1} - I_1\frac{f_1}{f_2}\right)\right). \end{aligned} \tag{25}$$

At this stage we can write the final expression for the Coriolis Hamiltonian (19),

$$H_{cor} = -i\,\frac{L_3}{\mathcal{F}^2}\Bigg(\cos\phi\,\left(I_2 f_2\,\frac{\partial}{\partial f_1} - I_1 f_1\,\frac{\partial}{\partial f_2}\right) + \left(I_2 - I_1 + \sin\phi\,\left[I_2\frac{f_2}{f_1} - I_1\frac{f_1}{f_2}\right]\right)\,\sin\phi\,\frac{\partial}{\partial\cos\phi} + (I_1 - I_2)\,\cot\phi\Bigg). \tag{26}$$

The rigid-body limit of Coriolis Hamiltonian can be obtained using (39) which yields

$$H_{cor}^{(eq)} = 0.$$

Thus, in the limit of zero vibrations the vibro-rotational couplings disappear. This fact is the inherent property of the Eckart BF which makes it so popular in molecular physics.

The expression (26) for the Coriolis Hamiltonian simplifies when the equilibrium inertia moments are equal $I = I_1 = I_2$,

$$H_{cor} = \frac{-i\,I}{\mathcal{F}^2}\,L_3\Bigg(\cos\phi\,\left(f_2\,\frac{\partial}{\partial f_1} - f_1\,\frac{\partial}{\partial f_2}\right) + \left(\frac{f_2}{f_1} - \frac{f_1}{f_2}\right)\,(\sin\phi)^2\,\frac{\partial}{\partial\cos\phi}\Bigg). \tag{27}$$

5 The rotational Hamiltonian

The rotational Hamiltonian expresses as [22,25]

$$H_{rot} = \frac{1}{2}\sum_{i,j=1}^{3}\mathcal{I}_{ij}L_i L_j, \tag{28}$$

where, as above, $L_i = (\mathbf{e}_i\cdot\mathbf{L})$ denotes the i-th component of the total angular momentum operator in BF and $\mathcal{I}$ is the effective inverse inertia tensor [22,25]. This tensor is symmetric

$$\mathcal{I}_{ij} = \mathcal{I}_{ji}.$$

The general expression for the tensor $\mathcal{I}$ for the Eckart frame has been derived in [23]. However, in that paper the closed form for H_{rot} in case of three particles was not given. The more detailed analysis presented in [25] makes it possible to derive a simpler form for the effective inertia tensor and, thereby, for the rotational Hamiltonian. In the three-

body problem the non-zero components of the effective inertia tensor $\mathcal{I}$ are [25]

$$\begin{aligned}
\mathcal{I}_{11} &= \frac{I_1}{\mathcal{F}^2}\left(1+\frac{f_1}{f_2\sin\phi}\right)^2+\frac{I_2(\cot\phi)^2}{\mathcal{F}^2},\\
\mathcal{I}_{22} &= \frac{I_2}{\mathcal{F}^2}\left(1+\frac{f_2}{f_1\sin\phi}\right)^2+\frac{I_1(\cot\phi)^2}{\mathcal{F}^2},\\
\mathcal{I}_{12} &= \frac{\cos\phi}{(\mathcal{F}\sin\phi)^2}\left((I_1+I_2)\sin\phi+I_1\frac{f_1}{f_2}+I_2\frac{f_2}{f_1}\right),\\
\mathcal{I}_{33} &= \frac{I_1+I_2}{\mathcal{F}^2}.
\end{aligned} \tag{29}$$

The rigid-body limit of the above expressions can be easily obtained noting Eq. (39). This leads to the well-known expression for the rotational Hamiltonian for a rotating planar rigid system

$$H_{rot}^{(eq)}=\frac{L_1^2}{2I_1}+\frac{L_2^2}{2I_2}+\frac{L_3^3}{2(I_1+I_2)}.$$

The equations (29) simplify in practically important case when two equilibrium moments of inertia are equal $I=I_1=I_2$,

$$\begin{aligned}
\mathcal{I}_{11} &= \frac{I}{(f_2\sin\phi)^2},\quad \mathcal{I}_{22}=\frac{I}{(f_1\sin\phi)^2},\\
\mathcal{I}_{12} &= \frac{I\cos\phi}{f_1f_2(\sin\phi)^2},\quad \mathcal{I}_{33}=\frac{2I}{\mathcal{F}^2}.
\end{aligned} \tag{30}$$

Thus, the rotational Hamiltonian can be written as

$$H_{rot}=\frac{I}{2(\sin\phi)^2}\left(\frac{L_1^2}{f_2^2}+\frac{L_2^2}{f_1^2}+\frac{\cos\phi}{f_1f_2}L_1L_2\right)+\frac{I\,L_3^2}{\mathcal{F}^2}. \tag{31}$$

This particularly simple expression has not yet been given in literature.

6 Conclusion

In the present paper the vibro-rotational decomposition of the three-body Hamiltonian has been analysed for the body-frame defined by the Eckart condition (5). The advantage of Eckart frame is that it minimises the vibro-rotational couplings (i.e. Coriolis part of the total Hamiltonian) for small amplitude vibrations. The geometrical explanation of the second Eckart condition (5) has been given in Sect. 2, see Fig. 2.

The derived expressions for the Coriolis (see Eq. (26) of Sect. 4) and rotational Hamiltonians (Eqs. (28), (29) of Sect. 5) are written in terms of Eckart internal coordinates which are connected (Appendix A) to conventional Jacobi-bond coordinates

widely used in three-body problem [1,24]. The expression for the vibrational Hamiltonian in terms of Eckart variables is given by Eq. (18). The use of the Eckart internal variables has made it possible to simplify the expressions for the vibro-rotational Hamiltonians.

It turns out that in the case of equal equilibrium inertia moments the Coriolis and rotational Hamiltonians can be written in particularly simple form, see Eqs. (27), (31), and (42), (43). Below the sum of Coriolis and rotational Hamiltonians is written explicitly in terms of mass-scaled Jacobi-bond coordinates,

$$H_{cor}+H_{rot}=\frac{-i}{F}L_3\left[\cos\theta\left(r_2\frac{\partial}{\partial r_1}-r_1\frac{\partial}{\partial r_2}\right)+\left(\frac{r_2}{r_1}-\frac{r_1}{r_2}\right)(\sin\theta)^2\frac{\partial}{\partial\cos\theta}\right]$$
$$+\frac{1}{2(\sin\theta)^2}\left(\frac{L_1^2}{r_2^2}+\frac{L_2^2}{r_1^2}+\frac{\cos\theta}{r_1r_2}L_1L_2\right)+\frac{L_3^2}{F}, \tag{32}$$

where the parameter F is defined by

$$F=r_1^2+r_2^2+2r_1r_2\sin\theta.$$

As one can easily see, the Coriolis term as well as the non-diagonal term of the rotational Hamiltonian vanish in the above expression in the limit $r_1\to r_2, \theta\to\pi/2$ which is the equilibrium configuration with two equal principal inertia moments. At the same time, the rotational Hamiltonian becomes that of a rotating rigid body.

For the sake of completeness we present here also the expression for the vibrational kinetic energy in terms of mass-scaled Jacobi-bond coordinates,

$$H_0=-\sum_{i=1}^{2}\frac{1}{2r_i^2}\frac{\partial}{\partial r_i}r_i^2\frac{\partial}{\partial r_i}-\frac{1}{2}\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\frac{\partial}{\partial\cos\theta}(\sin\theta)^2\frac{\partial}{\partial\cos\theta}+U(r_1,r_2,\cos\theta), \tag{33}$$

where U is the potential energy.

Appendix A: Relations between Eckart and Jacobi-bond coordinates

Below the connections between the set of Eckart and Jacobi internal coordinates are presented. Such connections follow from the definition of Eckart vectors (9) and the properties of the principal inertia axes. Omitting details of somewhat cumbersome computations we present here only the final results,

$$f_1^2=\frac{I_2}{I_1-I_2}\left(r_1^2(I_1-\rho_1^2)+r_2^2(I_1-\rho_2^2)-2(\mathbf{r}_1\cdot\mathbf{r}_2)\,(\boldsymbol{\rho}_1\cdot\boldsymbol{\rho}_2)\right). \tag{34}$$

For the vector $\mathbf{f}_2$ one has

$$f_2^2=\frac{-I_1}{I_1-I_2}\left(r_1^2(I_2-\rho_1^2)+r_2^2(I_2-\rho_2^2)-2(\mathbf{r}_1\cdot\mathbf{r}_2)\,(\boldsymbol{\rho}_1\cdot\boldsymbol{\rho}_2)\right), \tag{35}$$

The scalar product of Eckart vectors expresses as

$$(\mathbf{f}_1 \cdot \mathbf{f}_2) = \frac{|\boldsymbol{\rho}_1 \times \boldsymbol{\rho}_2|}{I_1 - I_2} \left((\boldsymbol{\rho}_1 \cdot \boldsymbol{\rho}_2)\,(r_1^2 - r_2^2) - (\mathbf{r}_1 \cdot \mathbf{r}_2)\,(\rho_1^2 - \rho_2^2) \right). \tag{36}$$

As is seen, the scalar product $(\mathbf{f}_1 \cdot \mathbf{f}_2)$ vanishes in the rigid-body limit when the vibration amplitudes tend to zero. The analysis of the rigid body limit of parameters f_1 and f_2 is slightly more complicated. Namely, in the rigid-body limit we have $\mathbf{r}_1 \to \boldsymbol{\rho}_1$ and $\mathbf{r}_2 \to \boldsymbol{\rho}_2$ which, noting the definitions (9), leads to

$$\left(f_1^2\right)_{eq} = x_1^2\rho_1^2 + x_2^2\rho_2^2 + 2x_1x_2(\boldsymbol{\rho}_1 \cdot \boldsymbol{\rho}_2). \tag{37}$$

Now we re-write ρ's in terms of their coordinates according to (8). This yields

$$\left(f_1^2\right)_{eq} = \left(x_1^2 + x_2^2\right)^2 + (x_1y_1 + x_2y_2)^2 = I_2^2. \tag{38}$$

Here, in the course of derivations we have utilized Eqs. (17) and (16).

Thus, in the limit of zero vibrations one has

$$\begin{aligned} (f_1)_{eq} &= I_2, \quad (f_2)_{eq} = I_1, \\ \phi_{eq} &= \frac{\pi}{2}. \end{aligned} \tag{39}$$

Clearly, the above Eqs. (34)–(36) are invalid when the equilibrium principal moments of inertia are equal. According to Eq. (44) of the next Appendix the condition $I_1 = I_2$ is met only if

$$\rho_1 = \rho_2, \quad \theta_e = \pi/2, \tag{40}$$

where θ_e is the mutual angle in the equilibrium configuration, see Fig. 1. Thus, the vectors $\boldsymbol{\rho}_1$ and $\boldsymbol{\rho}_2$ are perpendicular and, hence, we can choose them to define the Cartesian basis, i.e.

$$\mathbf{e}_1 = \frac{\boldsymbol{\rho}_1}{\rho_1}, \quad \mathbf{e}_2 = \frac{\boldsymbol{\rho}_2}{\rho_2}. \tag{41}$$

As a consequence we have that the coordinates in Eq. (8) become

$$x_1 = \rho_1, \quad y_2 = \rho_2, \quad x_2 = y_1 = 0.$$

From these identities and from (9) we obtain that at $I_1 = I_2$ the Eckart vectors can be chosen as

$$\mathbf{f}_1 = \rho\mathbf{r}_1, \quad \mathbf{f}_2 = \rho\mathbf{r}_2, \tag{42}$$

where $\rho = \rho_1 = \rho_2$. The corresponding Eckart parameter (12) expresses as

$$\mathcal{F}^2 = \rho^2 \left(r_1^2 + r_2^2 + 2r_1 r_2 \sin\theta\right). \tag{43}$$

Appendix B: The equilibrium inertia moments

The straightforward calculation of the eigenvalues of the inertia tensor leads to the following relations for the principal inertia moments of the equilibrium configuration

$$\begin{aligned} I_1 &= \frac{\rho_1^2 + \rho_2^2}{2} + \frac{1}{2}\sqrt{(\rho_1^2 - \rho_2^2)^2 + (2\rho_1\rho_2\cos\theta_e)^2}, \\ I_2 &= \frac{\rho_1^2 + \rho_2^2}{2} - \frac{1}{2}\sqrt{(\rho_1^2 - \rho_2^2)^2 + (2\rho_1\rho_2\cos\theta_e)^2}. \end{aligned} \tag{44}$$

We remind that $\rho_{1,2}$ are mass-scaled Jacobi vectors. To obtain expressions in terms of conventional Jacobi vectors one should apply the replacements $\rho_{1,2} \to \rho_{1,2}\sqrt{\mu}_{1,2}$ to the above Eq. (44).

As is seen from (44) the principal inertia moments are equal if Jacobi vectors are perpendicular (i.e. when $\theta_e = \pi/2$) and their lengths satisfy the equation

$$\mu_1 \rho_1^2 = \mu_2 \rho_2^2. \tag{45}$$

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