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Stratified dynamical systems and their boundary behaviour for three bodies in space, with insight into small vibrations

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Abstract

The centre-of-mass system for many particles is stratified into strata by the rotation group action. The principal stratum consists of nonlinear configurations. The collinear configurations form a lower dimensional stratum. Classical mechanics for many particles with nonlinear configurations and for those with collinear configurations are set up on the tangent or cotangent bundles over respective strata and can be reduced by the use of rotational symmetry. A question arises as to how a many-body system behaves in a neighbourhood of a collinear configuration. The system may make a vibration to bend its collinear configuration, which is a motion taking place across the boundary of the principal stratum. This paper deals with the behaviour of those boundaries for three bodies in space. The equations of motion for small vibrations as boundary behaviour at a collinear configuration will be given as a limit of those equations of motion for nonlinear configurations by means of two key facts: that the isotropy subgroup may act non-trivially on the tangent space at the collinear configuration and that vibrations take place in a constant plane in space. Further, the perturbation of small vibrations is studied by applying Moser's averaging method to show that small vibrations may give rise to finite rotations after a sufficiently large number of periods.

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1. Introduction

The centre-of-mass system for many particles is stratified into strata according to the orbit types of the rotation group action. The principal stratum consists of nonlinear configurations. The collinear configurations form a lower dimensional stratum, which is a boundary of the principal stratum. Quantum mechanics on the stratified centre-of-mass system has been discussed in [1].

Classical mechanics for many particles with nonlinear configurations and for those with collinear configurations are set up on the tangent or cotangent bundles over respective strata and can be reduced by the use of rotational symmetry [2]. A question arises as to how a many-body system behaves in a neighbourhood of a collinear configuration. The many-body system may make a vibration to bend its collinear configuration. This motion takes place across the lower dimensional stratum into the principal stratum. While each of the strata has a different number of local coordinates, how can one describe such a vibration in terms of local coordinates? This paper will deal with boundary motions such as small vibrations for a linear molecule, where a many-body system is called a linear or a nonlinear molecule, according to whether its stationary shape is collinear or nonlinear.

It is long since the theory of molecular vibrations was established (see [3], for example). However, linear molecules were not discussed. In 1970, Watson [4] tried to discuss the vibration–rotation Hamiltonian of linear molecules, but the boundary behaviour of a linear molecule is still an open question. As stated above, this paper is concerned with small vibrations of a linear molecule, since they are typical boundary behaviour of the linear molecule. For this purpose, we start with vibrational motions for nonlinear configurations and then deal with small deviations of a vibrational motion. For confirmation, we here give the definition of vibrational motions; a motion is called vibrational, if its total angular momentum vanishes. Small vibrations are then taken as small deviations at an equilibrium configuration, so that they are interpreted as taking place in the vibrational subspace (see (2.10) for definition) of the tangent space at the configuration. Since any 'small' neighbourhood of the origin of the vibrational subspace is, of course, imbedded into the centre-of-mass system, small vibrations are realized in the centre-of-mass system.

Keeping the above interpretation of small vibrations in mind, we study the boundary behaviour of a three-body system in particular. The spaces of nonlinear configurations and of collinear ones for a three-body system are of dimensions 6 and 4, respectively. Further, as is well known, in small vibrations of a triatomic molecule, there are four linearly independent vibration modes for a linear molecule, but only three modes for a nonlinear molecule. This well-known fact corresponds to the fact that the vibrational subspaces at a nonlinear configuration and at a collinear configuration are of dimensions 3 and 4, respectively. In the study of small vibrations of a linear triatomic molecule, the difference in the degrees of freedom and in the number of vibration modes should be taken into account and resolved consistently to provide the equations of small vibrations. There are two keys to the problem. One is the isotropy subgroup of the rotation group at a collinear configuration. The isotropy subgroup keeps the collinear configuration fixed, but acts non-trivially on the tangent space at the collinear configuration, and in particular on the vibrational subspace. The other is the mechanical fact that the vibration takes place in a constant plane in space. By means of these keys, it will be shown that the equations of small vibration for a linear triatomic molecule result from those for a nonlinear triatomic molecule as a limit along with some additional procedure. To be precise, three of the equations of small vibration are obtained by the limiting procedure, and another equation of small vibration takes the same form as one (a bending mode) of the three equations because of the symmetry.

Since vibrations may cause changes in configurations of the three-body system, a question arises as to whether small vibrations give rise to finite rotations or not. It is shown that a large number of periods of small vibrations may cause finite rotations, by applying Moser's averaging method [5] to the perturbation of small vibrations near an equilibrium for both a linear and a nonlinear molecule.

The organization of this paper is as follows: stratified dynamical systems are reviewed in section 2 in both the Lagrangian and the Hamiltonian formalisms. Section 3 deals with

vibrations and small vibrations. Moser's averaging method is reviewed, which will be applied in sections 5 and 6 to show the existence of a periodic solution as a perturbation of the small vibration of a triatomic molecule. Section 4 contains a review of three-body systems. Sections 5 and 6 are concerned with small vibrations of a nonlinear and a linear triatomic molecule, respectively. In particular, the equations of small vibrations for a linear triatomic molecule are obtained as a limit from those for a nonlinear molecule. It is shown further that small vibrations may give rise to finite rotations after a large number of periods of small vibrations. Section 7 contains remarks on the boundary behaviour in the shape space. In particular, how geodesics of the shape space behaves at the boundary of the shape space is discussed.

2. A review of stratified dynamical systems

This section is a review of stratified dynamical systems for many particles in space (see [2] for details). Let $\boldsymbol{x}_j \in \mathbf{R}^3$ and m_j denote the position vectors and the masses of N particles, respectively. The centre-of-mass system for N particles in space is then expressed as

$$M = \left\{ x = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) \,\middle|\, \sum_{j=1}^{N} m_j \boldsymbol{x}_j = 0 \right\}. \tag{2.1}$$

We introduce the Jacobi vectors, $\boldsymbol{r}_k$, $k = 1, \ldots, N-1$, by

$$\boldsymbol{r}_k := \left(\frac{1}{\mu_k} + \frac{1}{m_{k+1}} \right)^{-1/2} \left(\boldsymbol{x}_{k+1} - \frac{1}{\mu_k} \sum_{i=1}^{k} m_i \boldsymbol{x}_i \right), \qquad \mu_k := \sum_{i=1}^{k} m_i. \tag{2.2}$$

Then, the centre-of-mass system can be viewed as

$$M \cong \{ x = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{N-1}) | \boldsymbol{r}_k \in \mathbf{R}^3, k = 1, \ldots, N-1 \}, \tag{2.3}$$

and x as a $3 \times (N-1)$ matrix. The rotation group $SO(3)$ acts on M in a natural manner,

$$x \mapsto gx = (g\boldsymbol{r}_1, \ldots, g\boldsymbol{r}_{N-1}), \qquad g \in SO(3). \tag{2.4}$$

According to the orbit type of the group action, M is stratified into the union of strata,

$$M = \dot{M} \cup M_1 \cup M_0, \tag{2.5}$$

where $\dot{M}$ denotes the principal stratum which consists of x with rank $x \geqslant 2$, and M_1 and M_0 are strata consisting of x with rank $x = 1$ and of x with rank $x = 0$, respectively. The strata $\dot{M}$ and M_1 are interpreted as the spaces of nonlinear and of collinear configurations, respectively. The stratum M_0 describes the state that all the particles collide at the origin.

We denote by π the natural projection

$$\pi : M \longrightarrow M/SO(3), \tag{2.6}$$

where the base space $M/SO(3)$ is called the shape space. Since each stratum is invariant under the $SO(3)$ action, the projection (2.6) is also stratified into

$$\dot{M} \to \dot{M}/SO(3), \qquad M_1 \to M_1/SO(3), \qquad M_0 \to M_0/SO(3). \tag{2.7}$$

Classical Lagrangian systems are set up on $T(\dot{M})$ for nonlinear configurations and on $T(M_1)$ for collinear configurations, respectively. The respective Lagrangian systems are reduced by the use of rotational symmetry to respective systems defined on vector bundles over respective shape spaces $\dot{M}/SO(3)$ and $M_1/SO(3)$.

We first review the Lagrangian system on $T(\dot{M})$. The inertia tensor, $A_x : \mathbf{R}^3 \to \mathbf{R}^3$, is defined by

$$A_x(\boldsymbol{v}) = \sum_{k=1}^{N-1} \boldsymbol{r}_k \times (\boldsymbol{v} \times \boldsymbol{r}_k), \qquad \boldsymbol{v} \in \mathbf{R}^3, \tag{2.8}$$

and the connection form ω is defined for $x \in \dot{M}$ to be

$$\omega_x = R\left(A_x^{-1}\left(\sum_k \boldsymbol{r}_k \times \mathrm{d}\boldsymbol{r}_k\right)\right), \tag{2.9}$$

where $R : \mathbf{R} \to so(3)$ is the isomorphism defined by $R(\boldsymbol{a})\boldsymbol{x} = \boldsymbol{a} \times \boldsymbol{x}$ for $\boldsymbol{a}, \boldsymbol{x} \in \mathbf{R}^3$. Note that A_x^{-1} exists only for $x \in \dot{M}$. The connection form ω determines a direct sum decomposition of the tangent space $T_x(\dot{M})$;

$$T_x(\dot{M}) = V_x \oplus H_x, \tag{2.10}$$

where $V_x := T_x(\mathcal{O}_x)$, the tangent space to the orbit $\mathcal{O}_x$, and $H_x := \ker \omega_x$. Tangent vectors in V_x and in H_x are called vertical (or rotational) and horizontal (or vibrational), respectively. Further, V_x and H_x are orthogonal to each other with respect to the metric

$$\mathrm{d}s^2 = \sum_{k=1}^{N-1} \mathrm{d}\boldsymbol{r}_k \cdot \mathrm{d}\boldsymbol{r}_k. \tag{2.11}$$

We now introduce local coordinates to describe the equations of motion. Let $\sigma : U \to \dot{M}$ be a local section, where U is an open subset of $\dot{M}/SO(3)$. Then, any point $x \in \pi^{-1}(U)$ is put in the form

$$x = g\sigma(q) = (g\boldsymbol{\sigma}_1(q), \ldots, g\boldsymbol{\sigma}_{N-1}(q)), \qquad g \in SO(3), \quad q \in U. \tag{2.12}$$

We denote by (q^α) a system of local coordinates on U. In terms of local coordinates (q, g) on $\pi^{-1}(U) \cong U \times SO(3)$, the connection form is expressed as

$$\omega_{g\sigma(q)} = g(g^{-1}\,\mathrm{d}g + \omega_{\sigma(q)})g^{-1}, \tag{2.13}$$

where the form $\omega_{\sigma(q)}$ is defined and expressed as

$$\omega_{\sigma(q)} = R\left(A_{\sigma(q)}^{-1}\left(\sum_k \boldsymbol{\sigma}_k(q) \times \mathrm{d}\boldsymbol{\sigma}_k(q)\right)\right) \tag{2.14a}$$

$$= \sum_{\alpha=1}^{3N-6} \Lambda_\alpha(q)\,\mathrm{d}q^\alpha. \tag{2.14b}$$

We introduce the 1-forms Θ^a, $a = 1, 2, 3$, by putting

$$g^{-1}\,\mathrm{d}g + \omega_{\sigma(q)} = \sum_{a=1}^{3} \Theta^a R(\boldsymbol{e}_a). \tag{2.15}$$

Then the 1-forms $\mathrm{d}q^\alpha$ and Θ^a form a local basis of the space of 1-forms on $\pi^{-1}(U)$. According to the orthogonal decomposition (2.10), the metric (2.11) is broken up into the sum of vibrational and rotational parts:

$$\mathrm{d}s^2 = \sum_{\alpha,\beta} a_{\alpha\beta}\,\mathrm{d}q^\alpha\,\mathrm{d}q^\beta + \sum_{a,b} A_{ab}\Theta^a\Theta^b, \tag{2.16}$$

where $(a_{\alpha\beta})$ is the Riemannian metric projected from $\mathrm{d}s^2$ through π as a Riemannian submersion and (A_{ab}) are the components of $A_{\sigma(q)}$ with respect to the standard basis; $A_{ab} = \boldsymbol{e}_a \cdot A_{\sigma(q)}(\boldsymbol{e}_b)$.

Let $(q, g, \dot{q}, \dot{g})$ be local coordinates on $T(\pi^{-1}(U))$, where $(q, g) \in \pi^{-1}(U)$ and $\dot{q} = (\dot{q}^\alpha)$. In view of (2.15), we introduce an $so(3)$-valued variable Π and a vector-valued variable $\boldsymbol{\pi}$ by

$$\Pi = g^{-1}\dot{g} + \sum_{\alpha=1}^{3N-6} \Lambda_\alpha(q)\dot{q}^\alpha, \qquad R(\boldsymbol{\pi}) = \Pi, \tag{2.17}$$

respectively.

On the tangent bundle $T(\dot{M})$, a rotationally invariant Lagrangian is given by

$$L = \frac{1}{2}\sum_{\alpha,\beta} a_{\alpha\beta}\dot{q}^\alpha\dot{q}^\beta + \frac{1}{2}\sum_{a,b} A_{ab}\pi^a\pi^b - V(q), \tag{2.18}$$

where π^a are components of $\boldsymbol{\pi}$ and $V(q)$ denotes a potential function depending on $q \in \dot{M}/SO(3)$ only. By the use of rotational symmetry, the Euler–Lagrangian equations for L reduces to equations defined on the vector bundle $T(\dot{M}/SO(3)) \oplus \widetilde{\mathcal{G}}$, where $\widetilde{\mathcal{G}}$ denotes the adjoint bundle defined to be $\widetilde{\mathcal{G}} := \dot{M} \times_{SO(3)} \mathcal{G}$ with $\mathcal{G} = so(3)$. The reduced equations are given by

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\dot{q}^\alpha + \sum_{\beta,\gamma}\Gamma^\alpha_{\beta\gamma}\dot{q}^\beta\dot{q}^\gamma + \sum_\beta a^{\alpha\beta}\frac{\partial V}{\partial q^\beta} \\ = \sum_\beta a^{\alpha\beta}\left(\sum_\gamma A_{\sigma(q)}\boldsymbol{\pi}\cdot\boldsymbol{\kappa}_{\beta\gamma}\dot{q}^\gamma + \frac{1}{2}\boldsymbol{\pi}\cdot\left(\frac{\partial A_{\sigma(q)}}{\partial q^\beta} - [\Lambda_\beta, A_{\sigma(q)}]\right)\boldsymbol{\pi}\right),\end{aligned} \tag{2.19}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(A_{\sigma(q)}\boldsymbol{\pi}) = A_{\sigma(q)}\boldsymbol{\pi}\times\boldsymbol{\pi} - A_{\sigma(q)}\boldsymbol{\pi}\times\sum_\alpha \boldsymbol{\lambda}_\alpha\dot{q}^\alpha, \tag{2.20}$$

where $\Gamma^\alpha_{\beta\gamma}$ are the Christoffel symbols formed from the metric tensor $a_{\alpha\beta}$, and $(a^{\alpha\beta}) = (a_{\alpha\beta})^{-1}$, $\Lambda_\alpha = R(\boldsymbol{\lambda}_\alpha)$, and $K_{\alpha\beta} = R(\boldsymbol{\kappa}_{\alpha\beta})$ are the curvature tensors defined by

$$K_{\alpha\beta} := \frac{\partial\Lambda_\beta}{\partial q^\alpha} - \frac{\partial\Lambda_\alpha}{\partial q^\beta} - [\Lambda_\alpha, \Lambda_\beta]. \tag{2.21}$$

We note that equation (2.20) is equivalent to the conservation of the total angular momentum

$$\boldsymbol{L} = \sum_{j=1}^{N-1} \boldsymbol{r}_j \times \dot{\boldsymbol{r}}_j = gA_{\sigma(q)}\boldsymbol{\pi}. \tag{2.22}$$

In the Hamiltonian formalism, on introducing the variables p_α and $\boldsymbol{\mu}$ by

$$p_\alpha = \sum_\beta a_{\alpha\beta}\dot{q}^\beta, \qquad \boldsymbol{\mu} = A_{\sigma(q)}\boldsymbol{\pi}, \tag{2.23}$$

respectively, the equations of motion for the Hamiltonian

$$H = \frac{1}{2}\sum_{\alpha,\beta} a^{\alpha\beta}p_\alpha p_\beta + \frac{1}{2}\sum_{a,b} A^{ab}\mu_a\mu_b + V \tag{2.24}$$

with $(A^{ab}) = (A_{ab})^{-1}$ turn out to be given by

$$\frac{\mathrm{d}q^\alpha}{\mathrm{d}t} = \sum_\beta a^{\alpha\beta} p_\beta, \tag{2.25a}$$

$$\frac{\mathrm{d}p_\alpha}{\mathrm{d}t} = \sum_{\beta,\lambda,\mu} a^{\mu\beta}\Gamma^\lambda_{\beta\alpha} p_\lambda p_\mu - \frac{\partial V}{\partial q^\alpha} + \sum_{\beta,\gamma} \boldsymbol{\mu}\cdot\boldsymbol{\kappa}_{\alpha\beta} a^{\beta\gamma} p_\gamma - \frac{1}{2}\boldsymbol{\mu}\cdot\left(\frac{\partial A^{-1}_{\sigma(q)}}{\partial q^\alpha} - \left[\Lambda_\alpha, A^{-1}_{\sigma(q)}\right]\right)\boldsymbol{\mu}, \tag{2.25b}$$

$$\boldsymbol{\pi} = A^{-1}_{\sigma(q)}\boldsymbol{\mu}, \tag{2.26a}$$

$$\frac{\mathrm{d}\boldsymbol{\mu}}{\mathrm{d}t} = \boldsymbol{\mu}\times A^{-1}_{\sigma(q)}\boldsymbol{\mu} - \boldsymbol{\mu}\times\sum_{\alpha,\beta} a^{\alpha\beta} p_\alpha \boldsymbol{\lambda}_\beta. \tag{2.26b}$$

These equations are defined on the vector bundle $T^*(\dot{M}/SO(3)) \oplus \widetilde{\mathcal{G}}^*$, where $\widetilde{\mathcal{G}}^* := \dot{M}\times_{SO(3)}\mathcal{G}^*$ with $\mathcal{G}^* = so(3)^*$.

A Lagrangian and a Hamiltonian system for collinear configurations are defined on the tangent and the cotangent bundles, $T(M_1)$ and $T^*(M_1)$, respectively, and are reduced by the use of rotational symmetry. We do not give those equations of motion here (see [2]).

3. Vibrations and small vibrations

We restrict ourselves to vibrations which are defined to be motions having the vanishing total angular momentum $\boldsymbol{L} = gA_{\sigma(q)}\boldsymbol{\pi} = 0$. Since $A_{\sigma(q)}$ is non-degenerate for $\sigma(q)\in\dot{M}$, $\boldsymbol{L}=0$ implies $\boldsymbol{\pi}=0$, which is a trivial solution to the rotational part (2.20) of the equations of motion. Then the vibrational part (2.19) reduces to

$$\frac{\mathrm{d}}{\mathrm{d}t}\dot{q}^\alpha + \sum_{\beta,\gamma}\Gamma^\alpha_{\beta\gamma}\dot{q}^\beta\dot{q}^\gamma + \sum_\beta a^{\alpha\beta}\frac{\partial V}{\partial q^\beta} = 0. \tag{3.1}$$

If this equation is solved by $q(t)$, then the condition $\boldsymbol{\pi}=0$ is written out, in turn, as

$$\frac{\mathrm{d}g}{\mathrm{d}t} = -g\sum_\alpha \Lambda_\alpha(q(t))\dot{q}^\alpha, \tag{3.2}$$

which can be integrated to give $g(t)$. Then we obtain a vibrational motion $x(t) = g(t)\sigma(q(t))$ in $\dot{M}$. Note that since $\boldsymbol{L}=0$, one has $\dot{x}(t)\in H_{x(t)}$.

Let $\eta = (\eta^\alpha)$ be a variational vector along a solution $q(t)$ to (3.1). In the same method for obtaining the Jacobi equation for geodesic deviations, η is shown to be subject to the equation

$$\frac{\mathrm{D}^2\eta^\alpha}{\mathrm{d}t^2} + \sum_{\beta,\gamma,\mu} R_{\mu\beta\gamma}{}^\alpha \dot{q}^\beta\dot{q}^\gamma\eta^\mu + \sum_{\beta,\gamma} a^{\alpha\beta}H_{\gamma\beta}\eta^\gamma = 0, \tag{3.3}$$

where $\mathrm{D}/\mathrm{d}t$ denotes the covariant differentiation along the curve $q(t)$ with respect to the Riemannian metric $a_{\alpha\beta}$, and $R_{\mu\beta\gamma}{}^\alpha$ and $H_{\gamma\beta} := \nabla_\gamma\nabla_\beta V$ are, respectively, the components of the Riemann curvature tensor and the Hessian for V with ∇_α denoting the covariant differentiation (see [6]).

Let $q(t) = q_0$ be an equilibrium point, a special solution to (3.1) with $\frac{\partial V}{\partial q^\alpha}(q_0) = 0$. Then, the variational equation (3.3) reduces to

$$\frac{\mathrm{d}^2\eta^\alpha}{\mathrm{d}t^2} = -\sum_{\beta,\gamma} a^{\alpha\beta}(q_0)W_{\gamma\beta}\eta^\gamma, \qquad W_{\gamma\beta} := \frac{\partial^2 V}{\partial q^\gamma\partial q^\beta}(q_0). \tag{3.4}$$

Though $\eta = (\eta^\alpha) \in T_{q_0}(\dot{M}/SO(3))$, it can be horizontally lifted to $\widetilde{\eta} \in H_{x_0}$ with $x_0 \in \pi^{-1}(q_0)$. Since $\dot{M}$ is an open subset of the Euclidean space $M \cong \mathbf{R}^{3(N-1)}$, the $\widetilde{\eta}$ can be viewed as a small vibration about the equilibrium configuration x_0 in $\dot{M}$.

Apart from small vibrations, we make a remark on local coordinates in a neighbourhood U of q_0. Let $v_\alpha \in H_{x_0}$, $\alpha = 1, \ldots, 3N-6$, be orthonormal vibrational vectors at $x_0 \in \pi^{-1}(q_0)$. Take a geodesic $x(t) = x_0 + t\sum_\alpha c_\alpha v_\alpha$ with c_α constants, which describes a motion of free N particles. Since $\dot{x}(t) \in H_{x(t)}$, the $x(t)$ is a horizontal geodesic. It then projects to a geodesic $\pi(x(t))$ in U with respect to the Riemannian metric $(a_{\alpha\beta})$. Hence, one obtains

$$\pi(x(t)) = \exp_{q_0}\left(t\sum_\alpha c_\alpha \pi_*(v_\alpha)\right), \tag{3.5}$$

where exp and π_* denote the exponential map (see [7], for example) with respect to the Riemannian metric $(a_{\alpha\beta})$ and the differential map of π, respectively. Thus, the Cartesian coordinates η'_α in H_{x_0} with respect to the orthonormal frame v_α project to normal coordinates in the neighbourhood of q_0. Note that since the metric $(a_{\alpha\beta})$ on $\dot{M}/SO(3)$ is the one submersed from the Euclidean metric on $\dot{M}$, $\pi_*(v_\alpha)$ are orthonormal with respect to the metric $(a_{\alpha\beta})$ as well. An example will be given in section 5.

Conversely, the geodesic $\exp_{q_0} t\eta$ passing q_0 in the direction of $\eta \in T_{q_0}(\dot{M}/SO(3))$ at $t = 0$ can be horizontally lifted to $x(t) \in \dot{M}$ so as to pass an arbitrarily chosen point $x_0 \in \pi^{-1}(q_0)$. Since the geodesic $\exp_{q_0} t\eta$ is a free particle motion in $\dot{M}/SO(3)$, the lift $x(t)$ should be a straight line through x_0, a geodesic in M. The $(3N-6)$-dimensional plane, rather an open subset of it, spanned by those straight lines is called the Eckart section by Littlejohn *et al* [8, 9].

We now review variational equations in the Hamiltonian formalism according to [10]. For $\boldsymbol{\mu} = 0$, equation (2.25) reduces to

$$\frac{\mathrm{d}q^\alpha}{\mathrm{d}t} = \sum_\beta a^{\alpha\beta} p_\beta, \tag{3.6a}$$

$$\frac{\mathrm{d}p_\alpha}{\mathrm{d}t} = \sum_{\beta,\lambda,\mu} a^{\mu\beta}\Gamma^\lambda_{\beta\alpha} p_\lambda p_\mu - \frac{\partial V}{\partial q^\alpha}, \tag{3.6b}$$

which are the usual Hamilton's equation associated with the Hamiltonian

$$H = \frac{1}{2}\sum_{\alpha,\beta} a^{\alpha\beta} p_\alpha p_\beta + V. \tag{3.7}$$

We introduce a local frame E_α, F^α on the cotangent bundle $T^*(\dot{M}/SO(3))$ by

$$E_\alpha = \frac{\partial}{\partial q^\alpha} + \sum_{\beta,\gamma} p_\beta \Gamma^\beta_{\alpha\gamma}\frac{\partial}{\partial p_\gamma}, \qquad F^\alpha = \frac{\partial}{\partial p_\alpha}. \tag{3.8}$$

Let

$$Y = \sum_\alpha \eta^\alpha E_\alpha + \sum_\alpha \zeta_\alpha F^\alpha \tag{3.9}$$

be a vector field defined along a solution $(q(t), p(t))$ to (3.6). If Y is a variational vector, it is required to leave equation (3.6) invariant infinitesimally. It then turns out that Y should satisfy

$$\frac{\mathrm{d}\eta^\alpha}{\mathrm{d}t} = -\sum_{\beta,\gamma}\Gamma^\alpha_{\beta\gamma}\dot{q}^\gamma\eta^\beta + \sum_\beta a^{\alpha\beta}\zeta_\beta, \tag{3.10a}$$

$$\frac{\mathrm{d}\zeta_\alpha}{\mathrm{d}t} = -\sum_{\beta,\lambda,\mu} R_{\beta\lambda\mu\alpha}\dot{q}^\lambda\dot{q}^\mu\eta^\beta + \sum_{\beta,\gamma}\Gamma^\beta_{\alpha\gamma}\dot{q}^\gamma\zeta_\beta - \sum_\beta H_{\beta\alpha}\eta^\beta, \tag{3.10b}$$

where $\dot{q}^\alpha = \sum_\beta a^{\alpha\beta}p_\beta$ and $H_{\alpha\beta}$ denotes the Hessian already introduced.

For an equilibrium point $(q_0, 0)$ with $\frac{\partial V}{\partial q^\alpha}(q_0) = 0$, the above equations reduce to

$$\frac{\mathrm{d}\eta^\alpha}{\mathrm{d}t} = \sum_\beta a^{\alpha\beta}\zeta_\beta, \tag{3.11a}$$

$$\frac{\mathrm{d}\zeta_\alpha}{\mathrm{d}t} = -\sum_\beta W_{\beta\alpha}\eta^\beta, \tag{3.11b}$$

where $a^{\alpha\beta}$ and $H_{\beta\alpha} = W_{\beta\alpha}$ should be evaluated at q_0. These are equivalent to (3.4), of course.

In what follows, we discuss a perturbation of (3.11). We assume that the equilibrium point $(q_0, 0)$ is stable, and that solutions to (3.11) are all periodic with the same period. Then, equations (3.11) are viewed as the equations of motion for the harmonic oscillator, and the Hamiltonian (3.7) is looked upon as a perturbation of that for the harmonic oscillator.

We are now in a position to apply Moser's averaging method for periodic motions [5, 11]. According to [5], a procedure for finding periodic solutions near an equilibrium is as follows: let H be a perturbed Hamiltonian, $H = H_2 + \varepsilon H_3 + \cdots$, where H_p is a homogeneous polynomial of degree p in $(x, y) \in \mathbf{R}^n \times \mathbf{R}^n$, and where the orbits of the Hamiltonian flow, ϕ_t, associated with H_2 are assumed to have all period 2π. By stretching the variables $x \to \varepsilon x$, $y \to \varepsilon y$, one can reduce the problem to a level surface $M_E := H_2^{-1}(E)$ with E a positive constant. The perturbation function will be H_4. Its average

$$\overline{H}_4 = \frac{1}{2\pi}\int_0^{2\pi} \phi_t^* H_4\,\mathrm{d}t \tag{3.12}$$

is defined on the orbit space, $\overline{M}_E := M_E/S^1$, where S^1 stands for the group determined by ϕ_t. We denote the projection by $\Pi : M_E \to \overline{M}_E$. Then, for every non-degenerate critical point $\overline{p} \in \overline{M}_E$ of $\overline{H}_4$, there exists a periodic solution to Hamilton's equations of motion for the perturbed Hamiltonian H in a neighbourhood of $\Pi^{-1}(\overline{p})$. We have to note that the level surface M_E is diffeomorphic with S^{2n-1}, so that the orbit space M_E/S^1 is diffeomorphic with $\mathbf{C}P^{n-1}$. Since the Euler characteristic of $\mathbf{C}P^{n-1}$ is n, the averaged Hamiltonian $\overline{H}_4$ on the orbit space has non-degenerate critical points, if $\overline{H}_4$ is regular. Thus, there exist periodic solutions, in general, for H.

According to this procedure, equation (3.6) will admit a periodic solution to the extent that the Hamiltonian (3.7) can be viewed as a perturbation of that for the harmonic oscillator in a neighbourhood of $(q_0, 0)$. If the potential function is chosen suitably, this will be the case.

For these periodic solutions $q(t)$, equation (3.2) will give rise to finite rotations, if integrated. In fact, the vibrational motion $x(t) = g(t)\sigma(q(t))$, $0 \leqslant t \leqslant T$, with $q(0) = q(T)$ yields a finite rotation $g(T)g(0)^{-1}$. Even if $g(t)g(0)^{-1}$ is a small but finite rotation, after a sufficiently large number of periods, $0 \leqslant t \leqslant nT$, the rotation $g(nT)g(0)^{-1}$ may become big, where n is the number of periods. In the following sections, we will apply this procedure to a three-body system to show that small vibrations may give rise to finite rotations in the centre-of-mass system.

4. Three-body systems

We are interested in the behaviour of many particles around collinear configurations. To observe such behaviour in an explicit manner, we treat a three-body system in particular. This

section is a review of three-body systems [2]. For a three-body system, the Jacobi vectors are given by

$$\boldsymbol{r}_1 = \sqrt{\frac{m_1 m_2}{m_1 + m_2}}(\boldsymbol{x}_2 - \boldsymbol{x}_1), \tag{4.1a}$$

$$\boldsymbol{r}_2 = \sqrt{\frac{m_3(m_1 + m_2)}{m_1 + m_2 + m_3}}\left(\boldsymbol{x}_3 - \frac{m_1\boldsymbol{x}_1 + m_2\boldsymbol{x}_2}{m_1 + m_2}\right). \tag{4.1b}$$

Note that $x = (\boldsymbol{r}_1, \boldsymbol{r}_2) \in \dot{M} \Leftrightarrow \operatorname{rank} x \geqslant 2$ and that $x = (\boldsymbol{r}_1, \boldsymbol{r}_2) \in M_1 \Leftrightarrow \operatorname{rank} x = 1$. Using the Jacobi vectors, we introduce shape (or internal) coordinates by

$$q_1 = r_1, \qquad q_2 = r_2 \cos\varphi, \qquad q_3 = r_2 \sin\varphi, \tag{4.2}$$

where

$$r_1 = \|\boldsymbol{r}_1\|, \qquad r_2 = \|\boldsymbol{r}_2\|, \qquad \boldsymbol{r}_1 \cdot \boldsymbol{r}_2 = r_1 r_2 \cos\varphi. \tag{4.3}$$

We note here that we have chosen to describe the coordinates with subscript indices.

We define a local section $\sigma(q) = (\boldsymbol{\sigma}_1(q), \boldsymbol{\sigma}_2(q))$ by

$$\boldsymbol{\sigma}_1(q) = q_1\boldsymbol{e}_3, \qquad \boldsymbol{\sigma}_2(q) = q_2\boldsymbol{e}_3 + q_3\boldsymbol{e}_1. \tag{4.4}$$

For a nonlinear molecule, the local section σ is defined originally in an open subset U of $\dot{M}/SO(3)$, so that q_1 and q_3 have to be restricted to positive real numbers. However, we take (q_1, q_2, q_3) as local coordinates beyond U,

$$\{(q_1, q_2, q_3) | q_1 \geqslant 0, q_3 \geqslant 0\}. \tag{4.5}$$

Then, we obtain a collinear shape if $q_3 = 0$, and the state that two of three particles collide but the remainder is separate, if $q_1 = 0$. If $q_1 = q_2 = q_3 = 0$, we have a triple collision. The three-body configurations are then described as $x = g\sigma(q)$, where $g \in SO(3)$. If we put $g = \mathrm{e}^{\phi R(\boldsymbol{e}_3)}\,\mathrm{e}^{\theta R(\boldsymbol{e}_2)}\,\mathrm{e}^{\psi R(\boldsymbol{e}_3)}$ in terms of the Euler angles, the local coordinates of $\dot{M}$ and of M_1 are given by $(q_1, q_2, q_3, \phi, \theta, \psi)$ and by (q_1, q_2, ϕ, θ), respectively. If we operate $\sigma(q)$ with $\mathrm{e}^{\psi R(\boldsymbol{e}_3)}$, the configurations $g\sigma(q) = (\boldsymbol{r}_1, \boldsymbol{r}_2)$ are expressed as

$$\boldsymbol{r}_1 = \mathrm{e}^{\phi R(\boldsymbol{e}_3)}\,\mathrm{e}^{\theta R(\boldsymbol{e}_2)} q_1\boldsymbol{e}_3, \tag{4.6a}$$

$$\boldsymbol{r}_2 = \mathrm{e}^{\phi R(\boldsymbol{e}_3)}\,\mathrm{e}^{\theta R(\boldsymbol{e}_2)}(q_2\boldsymbol{e}_3 + q_3\cos\psi\,\boldsymbol{e}_1 + q_3\sin\psi\,\boldsymbol{e}_2). \tag{4.6b}$$

As is easily observed from this, a nonlinear configuration tends to a collinear configuration, if $q_3 \to 0$.

In the following, we line up the quantities needed for studying the behaviour of the three-body system. The inertial tensor and its inverse at $\sigma(q)$ is given by

$$A_{\sigma(q)} = \begin{pmatrix} q_1^2 + q_2^2 & 0 & -q_1 q_2 \\ 0 & q_1^2 + q_2^2 + q_3^2 & 0 \\ -q_2 q_3 & 0 & q_3^2 \end{pmatrix}, \tag{4.7}$$

$$A^{-1}_{\sigma(q)} = \begin{pmatrix} \frac{1}{q_1^2} & 0 & \frac{q_2}{q_1^2 q_3} \\ 0 & \frac{1}{q_1^2+q_2^2+q_3^2} & 0 \\ \frac{q_2}{q_1^2 q_3} & 0 & \frac{q_1^2+q_2^2}{q_1^2 q_3^2} \end{pmatrix}, \tag{4.8}$$

respectively. The connection form is expressed as

$$\omega_{\sigma(q)} = \frac{q_2\,\mathrm{d}q_3 - q_3\,\mathrm{d}q_2}{q_1^2+q_2^2+q_3^2} R(\boldsymbol{e}_2), \tag{4.9}$$

which gives also the components $\Lambda_\alpha = R(\boldsymbol{\lambda}_\alpha)$ of $\omega_{\sigma(q)} = \sum \Lambda_\alpha\,\mathrm{d}q_\alpha$. We observe from these equations that $A_{\sigma(q)}$ is degenerate for $q_3 = 0$, and hence $A^{-1}_{\sigma(q)}$ is not defined for $q_3 = 0$. In spite of this fact, the $\Lambda_\alpha(q)$ has a limit as $q_3 \to 0$. The metric tensor and its inverse are given by

$$(a_{\alpha\beta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{q_1^2+q_2^2}{q_1^2+q_2^2+q_3^2} & \frac{q_2q_3}{q_1^2+q_2^2+q_3^2} \\ 0 & \frac{q_2q_3}{q_1^2+q_2^2+q_3^2} & \frac{q_1^2+q_3^2}{q_1^2+q_2^2+q_3^2} \end{pmatrix}, \tag{4.10}$$

$$(a^{\alpha\beta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{q_1^2+q_3^2}{q_1^2} & -\frac{q_2q_3}{q_1^2} \\ 0 & -\frac{q_2q_3}{q_1^2} & \frac{q_1^2+q_2^2}{q_1^2} \end{pmatrix}, \tag{4.11}$$

respectively. We observe also from the above equations that for $q_3 = 0$ the metric tensor and its inverse remain non-degenerate. The top-left 2×2 submatix of (4.10) with $q_3 = 0$ gives the metric on $M_1/SO(3)$.

We have already shown [2] that if the constraints, $q_3 = 0, \pi_3 = 0, q_1\dot{q}_2 - q_2\dot{q}_1 = 0$ are satisfied, and if the potential is such that $\frac{\partial V}{\partial q_3} = 0$ at $q_3 = 0$, the equations of motion for a nonlinear triatomic molecule reduce to those for a linear triatomic molecule.

5. Nonlinear triatomic molecules

This section is concerned with small vibrations of a nonlinear triatomic molecule near an equilibrium. We show that if all small vibrations have the same period 2π, the nonlinear triatomic molecule is allowed to have a perturbed but still periodic motion in the shape space $\dot{M}/SO(3)$, and further that the periodic motion gives rise to a finite rotation in $\dot{M}$.

The Jacobi vectors for the three-body system were given by (4.1) in terms of position vectors. Conversely, the position vectors are described as follows:

$$\boldsymbol{x}_1 = -N_1m_2\boldsymbol{r}_1 - N_2m_3\boldsymbol{r}_2, \tag{5.1a}$$

$$\boldsymbol{x}_2 = N_1m_1\boldsymbol{r}_1 - N_2m_3\boldsymbol{r}_2, \tag{5.1b}$$

$$\boldsymbol{x}_3 = N_2(m_1+m_2)\boldsymbol{r}_2, \tag{5.1c}$$

where

$$N_1 = (m_2m_1(m_1+m_2))^{-1/2}, \qquad N_2 = (m_3(m_1+m_2)(m_1+m_2+m_3))^{-1/2}. \tag{5.2}$$

Now, we take a fixed configuration $x_0 = (\boldsymbol{r}_1, \boldsymbol{r}_2) = (a\boldsymbol{e}_3, b\boldsymbol{e}_1)$ with $a, b > 0$, which is assumed to be an equilibrium configuration of a molecule in question. We are to study small vibrations of this molecule at x_0. A basis of the rotational subspace $V_{x_0} = T_{x_0}\big(\mathcal{O}_{x_0}\big)$ at $x_0 = (a\boldsymbol{e}_3, b\boldsymbol{e}_1)$ is given by

$$u_1 = R(\boldsymbol{e}_1)(a\boldsymbol{e}_3, b\boldsymbol{e}_1) = (-a\boldsymbol{e}_2, 0), \tag{5.3a}$$

$$u_2 = R(\boldsymbol{e}_2)(a\boldsymbol{e}_3, b\boldsymbol{e}_1) = (a\boldsymbol{e}_1, -b\boldsymbol{e}_3), \tag{5.3b}$$

$$u_3 = R(\boldsymbol{e}_3)(a\boldsymbol{e}_3, b\boldsymbol{e}_1) = (0, b\boldsymbol{e}_2). \tag{5.3c}$$

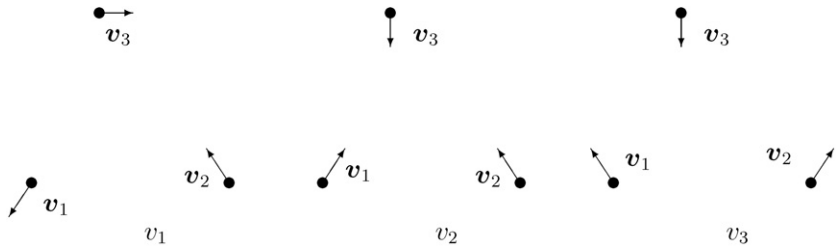

Figure 1. Vibrational vectors at a nonlinear configuration. The plane in which the molecule lies is the e_3–e_1 plane.

Vibrational vectors are those which are orthogonal to all the rotational vectors. We can take three of them as

$$v_1 = (be_1, ae_3), \tag{5.4a}$$

$$v_2 = (-be_3, -ae_1), \tag{5.4b}$$

$$v_3 = (ae_3, -be_1), \tag{5.4c}$$

which form an orthogonal basis of $H_{x_0} := V_{x_0}^{\perp}$.

We show that the vibrational vectors $v_\alpha, \alpha = 1, 2, 3$, are realized as so-called normal modes for the small vibration of a nonlinear triatomic molecule. To this end, we note that the tangent vectors $\dot{\boldsymbol{x}}_k$ and $\dot{\boldsymbol{r}}_j$ are related by equations similar to (5.1). Then, the component tangent vectors $\boldsymbol{v}_k := \dot{\boldsymbol{x}}_k$ for the vibrational vectors $v_\alpha, \alpha = 1, 2, 3$, are given, respectively, by

$$v_1; \begin{cases} \boldsymbol{v}_1 = -N_1 m_2 b\boldsymbol{e}_1 - N_2 m_3 a\boldsymbol{e}_3, \\ \boldsymbol{v}_2 = N_1 m_1 b\boldsymbol{e}_1 - N_2 m_3 a\boldsymbol{e}_3, \\ \boldsymbol{v}_3 = N_2(m_1 + m_2)a\boldsymbol{e}_3, \end{cases} \tag{5.5a}$$

$$v_2; \begin{cases} \boldsymbol{v}_1 = N_1 m_2 b\boldsymbol{e}_3 + N_2 m_3 a\boldsymbol{e}_1, \\ \boldsymbol{v}_2 = -N_1 m_1 b\boldsymbol{e}_3 + N_2 m_3 a\boldsymbol{e}_1, \\ \boldsymbol{v}_3 = -N_2(m_1 + m_2)a\boldsymbol{e}_1, \end{cases} \tag{5.5b}$$

$$v_3; \begin{cases} \boldsymbol{v}_1 = -N_1 m_2 a\boldsymbol{e}_3 + N_2 m_3 b\boldsymbol{e}_1, \\ \boldsymbol{v}_2 = N_1 m_1 a\boldsymbol{e}_3 + N_2 m_3 b\boldsymbol{e}_1, \\ \boldsymbol{v}_3 = -N_2(m_1 + m_2)b\boldsymbol{e}_1. \end{cases} \tag{5.5c}$$

These are shown in figure 1, describing vibration modes. We have to remark here that no equations of small vibration have been used to obtain these vibration modes. It is to be noted further that the choice of v_α is not unique. Another orthogonal basis of H_{x_0}, $(v_1', v_2', v_3') = (v_1, v_2, v_3)G$ with $G \in O(3)$, serves as normal modes for small vibrations. The choice of the basis of H_{x_0} may be determined by the potential function.

Since the centre-of-mass system is Euclidean, open subsets of H_{x_0} containing the origin of H_{x_0} is viewed as being immersed in $\dot{M}$. Vibrational small displacements at x_0 are then expressed as and given by

$$(\delta\boldsymbol{r}_1, \delta\boldsymbol{r}_2) = \varepsilon \sum_{\alpha=1}^{3} \eta_\alpha' v_\alpha \tag{5.6}$$

$$= \varepsilon((-b\eta_2' + a\eta_3')\boldsymbol{e}_3 + b\eta_1'\boldsymbol{e}_1, a\eta_1'\boldsymbol{e}_3 + (-a\eta_2' - b\eta_3')\boldsymbol{e}_1), \tag{5.7}$$

where ε is an infinitesimal parameter, and η'_α denote the Cartesian coordinates of H_{x_0}, but scaled by $\sqrt{a^2+b^2}$. We have found that the variational small displacement is put in the form

$$\delta \boldsymbol{r}_1 = \varepsilon((-b\eta'_2 + a\eta'_3)\boldsymbol{e}_3 + b\eta'_1\boldsymbol{e}_1), \qquad \delta \boldsymbol{r}_2 = \varepsilon(a\eta'_1\boldsymbol{e}_3 + (-a\eta'_2 - b\eta'_3)\boldsymbol{e}_1). \tag{5.8}$$

We now move to the tangent space $T_{\pi(x_0)}(\dot{M}/SO(3)) = \pi_* H_{x_0}$. We note first that, when projected, (η'_α) serve as local coordinates in a neighbourhood of $\pi(x_0)$. From (4.4), $\pi(x_0)$ is described as $(q_1, q_2, q_3) = (a, 0, b)$. We denote by $\delta q_\alpha := \varepsilon\eta_\alpha, \alpha = 1, 2, 3$, the small increment of the local coordinates q_α at $(q_1, q_2, q_3) = (a, 0, b)$. We wish to find the relation between η'_α and η_α. To this end, we recall that the local coordinates q_α are expressed as

$$q_1 = |\boldsymbol{r}_1|, \qquad q_2 = \boldsymbol{r}_1 \cdot \boldsymbol{r}_2/|\boldsymbol{r}_1|, \qquad q_3 = |\boldsymbol{r}_1 \times \boldsymbol{r}_2|/|\boldsymbol{r}_1|. \tag{5.9}$$

Differentiating these equations provides each of the infinitesimal increments δq_α at $(a, 0, b)$ in terms of $\delta \boldsymbol{r}_1, \delta \boldsymbol{r}_2$. Putting them together with (5.8) results in

$$\eta_1 = -b\eta'_2 + a\eta'_3, \tag{5.10a}$$

$$\eta_2 = \left(\frac{a^2+b^2}{a}\right)\eta'_1, \tag{5.10b}$$

$$\eta_3 = a\eta'_2 + b\eta'_3. \tag{5.10c}$$

We have thus obtained two local coordinate systems, (η_α) and (η'_α), in a neighbourhood of $\pi(x_0)$ along with the transformation rule (5.10).

We now assume that small vibrations are driven by the potential function given by

$$V' = \frac{\varepsilon^2}{2}\sum_\alpha \kappa_\alpha^2 (\eta'_\alpha)^2, \tag{5.11}$$

where κ_α are constants. This is because v_α are regarded as normal modes for small vibrations within a factor $\sqrt{a^2+b^2}$, so that the original potential function V is approximated by the quadratic function of the form (5.11) in a neighbourhood of $q_0 = \pi(x_0)$.

From (4.10), the metric tensor $(a_{\alpha\beta})$ is given, at $(q_1, q_2, q_3) = (a, 0, b)$, by

$$G := (a_{\alpha\beta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{a^2}{a^2+b^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5.12}$$

Then, the equation of small vibration (3.4) is expressed, in vector form, as

$$\frac{\mathrm{d}^2\eta}{\mathrm{d}t^2} = -G^{-1}W\eta, \qquad W = \left(\frac{\partial^2 V}{\partial q_\alpha \partial q_\beta}(q_0)\right), \tag{5.13}$$

which is diagonalized in the coordinates η'_α:

$$\frac{\mathrm{d}^2\eta'}{\mathrm{d}t^2} = -G'^{-1}W'\eta', \qquad G'^{-1}W' = \frac{1}{a^2+b^2}\,\mathrm{diag}\big(\kappa_1^2, \kappa_2^2, \kappa_3^2\big), \tag{5.14}$$

where use has been made of the transformation laws

$$G = M^T G' M, \qquad W = M^T W' M, \qquad M := \left(\frac{\partial \eta'_\alpha}{\partial \eta_\lambda}\right) = \frac{1}{a^2+b^2}\begin{pmatrix} 0 & a & 0 \\ -b & 0 & -a \\ a & 0 & -b \end{pmatrix}. \tag{5.15}$$

In the Hamiltonian formalism, the equation of small vibration (3.11) is put in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\eta \\ \zeta\end{pmatrix} = \begin{pmatrix} 0 & G^{-1} \\ -W & 0 \end{pmatrix}\begin{pmatrix}\eta \\ \zeta\end{pmatrix}, \qquad (\eta, \zeta) \in \mathbf{R}^3 \times \mathbf{R}^3. \tag{5.16}$$

Since (η', ζ') and (η, ζ) are subject to the transformation

$$\eta' = M\eta, \qquad \zeta' = (M^T)^{-1}\zeta, \tag{5.17}$$

the above equation is brought into the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\eta'\\ \zeta'\end{pmatrix} = \begin{pmatrix}0 & G'^{-1}\\ -W' & 0\end{pmatrix}\begin{pmatrix}\eta'\\ \zeta'\end{pmatrix}, \tag{5.18a}$$

$$G'^{-1} = \frac{1}{a^2+b^2}I, \qquad W' = \operatorname{diag}\bigl(\kappa_1^2, \kappa_2^2, \kappa_3^2\bigr), \tag{5.18b}$$

where I denotes the 3×3 unit matrix.

We wish to show that equation (3.6) as a perturbed equation of (5.16) admits a periodic solution by following Moser's procedure with the assumption that

$$\kappa_1^2 = \kappa_2^2 = \kappa_3^2 = a^2 + b^2. \tag{5.19}$$

With this assumption, equation (5.18) gives rise to the S^1 action,

$$\phi_t : \begin{pmatrix}\eta'(t)\\ \zeta'(t)\end{pmatrix} = \begin{pmatrix}\cos t I & \frac{\sin t}{a^2+b^2}I\\ -(a^2+b^2)\sin t I & \cos t I\end{pmatrix}\begin{pmatrix}\eta'(0)\\ \zeta'(0)\end{pmatrix}. \tag{5.20}$$

We have two local coordinate systems, $(\eta_\alpha, \zeta_\alpha)$ and $(\eta'_\alpha, \zeta'_\alpha)$, in a neighbourhood of $(q_0, 0) \in T^*(U)$. The local coordinates (q_α, p_α) are related to $(\eta_\alpha, \zeta_\alpha)$ by

$$(q_1, q_2, q_3) = (a, 0, b) + \varepsilon(\eta_1, \eta_2, \eta_3), \qquad (p_1, p_2, p_3) = \varepsilon(\zeta_1, \zeta_2, \zeta_3), \tag{5.21}$$

and $(\eta_\alpha, \zeta_\alpha)$ and $(\eta'_\alpha, \zeta'_\alpha)$ are subject to the transformation (5.17). We now assume that the potential function is given, as a perturbation of (5.11), by

$$V = \frac{\varepsilon^2}{2}\sum_\alpha (a^2+b^2)\eta_\alpha'^2 + \varepsilon^4\lambda\eta_1'^2\eta_2'\eta_3', \tag{5.22}$$

where λ is a parameter to be determined later. We now expand the Hamiltonian (3.7) in the coordinates $(\eta'_\alpha, \zeta'_\alpha)$, where $(a^{\alpha\beta})$ and V are given by (4.11) and by (5.22), respectively. A calculation results in

$$\varepsilon^{-2}H = H_2 + \varepsilon H_3 + \varepsilon^2 H_4 + O(\varepsilon^3), \tag{5.23}$$

where

$$H_2 = \frac{1}{2}\left((a^2+b^2)\sum_\alpha \eta_\alpha'^2 + \frac{1}{a^2+b^2}\sum_\alpha \zeta_\alpha'^2\right), \tag{5.24a}$$

$$H_3 = \frac{b}{a^2(a^2+b^2)^2}(-a((a^2-b^2)\eta_2' + 2ab\eta_3')\zeta_1'^2 + (a^2+b^2)\eta_1'\zeta_1'(a\zeta_2' + b\zeta_3')), \tag{5.24b}$$

$$\begin{aligned} H_4 = \frac{a}{2a^4(a^2+b^2)^2}\bigl(&a^2((a^2-b^2)\eta_2' + 2ab\eta_3')((a^2-3b^2)\eta_2' + 4ab\eta_3')\zeta_1'^2\\ &- 2a(a^2+b^2)\eta_1'\zeta_1'((a^2-2b^2)\eta_2' + 3ab\eta_3')(a\zeta_2' + b\zeta_3')\\ &+ (a^2+b^2)^2\eta_1'^2(a\zeta_2' + b\zeta_3')^2\bigr) + \lambda\eta_1'^2\eta_2'\eta_3'. \end{aligned} \tag{5.24c}$$

Let E be a positive number. The level surface $H_2^{-1}(E)$ is diffeomorphic with a sphere S^5, on which the S^1 action (5.20) is defined. It is easy to show that the following functions are invariant under the S^1 action ϕ_t,

$$E_{\alpha\beta} = (a^2+b^2)\eta_\alpha'\eta_\beta' + \frac{\zeta_\alpha'\zeta_\beta'}{a^2+b^2}, \tag{5.25}$$

$$L_{\alpha\beta} = \eta'_\alpha \zeta'_\beta - \zeta'_\alpha \eta'_\beta. \tag{5.26}$$

These invariants satisfy the relations

$$E_{\alpha\beta}E_{\mu\nu} = E_{\alpha\mu}E_{\beta\nu} + L_{\alpha\nu}L_{\beta\mu}, \tag{5.27}$$

and

$$E = E_{11} + E_{22} + E_{33} \qquad \text{on} \quad H_2^{-1}(E). \tag{5.28}$$

We now average the functions H_2, H_3, H_4. Let

$$\overline{H}_p := \frac{1}{2\pi}\int_0^{2\pi} \phi_t^* H_p \,\mathrm{d}t. \tag{5.29}$$

One can easily obtain

$$\overline{H}_2 = \tfrac{1}{2}(E_{11} + E_{22} + E_{33}), \qquad \overline{H}_3 = 0. \tag{5.30}$$

Using the formulae

$$\frac{1}{2\pi}\int_0^{2\pi} \phi_t^*(\eta'_\alpha\eta'_\beta\eta'_\mu\eta'_\nu)\,\mathrm{d}t = \frac{1}{8(a^2+b^2)^2}(E_{\alpha\beta}E_{\mu\nu} + E_{\alpha\mu}E_{\beta\nu} + E_{\alpha\nu}E_{\beta\mu}), \tag{5.31}$$

$$\frac{1}{2\pi}\int_0^{2\pi} \phi_t^*(\eta'_\alpha\eta'_\beta\zeta'_\mu\zeta'_\nu)\,\mathrm{d}t = \frac{1}{8}(E_{\alpha\beta}E_{\mu\nu} + 2L_{\alpha\mu}L_{\beta\nu} - L_{\alpha\beta}L_{\mu\mu}), \tag{5.32}$$

we average H_4 to obtain

$$\begin{aligned}\overline{H}_4 = {} & \frac{1}{16a^4(a^2+b^2)^2}\big(b^2E_{11}(8a^2b^2E_{22} - 2ab(7a^2+3b^2)E_{23} + (3a^4 - 4a^2b^2 + b^4)E_{33}) \\ & + 2\big(4a^2(a^2-b^2)L_{21}^2 + 2ab(8a^4 - a^2b^2 - b^4)L_{21}L_{31} \\ & + b^2(15a^4 + 8a^2b^2 + b^4)L_{31}^2\big)\big) + \frac{\lambda}{8(a^2+b^2)^2}(3E_{11}E_{23} - 2L_{21}L_{31}).\end{aligned} \tag{5.33}$$

If we set

$$\lambda = \frac{b^3(7a^2+3b^2)}{3a^3}, \tag{5.34}$$

we have $\overline{H}_4$ expressed as

$$\begin{aligned}\overline{H}_4 = {} & \frac{1}{16a^4(a^2+b^2)^2}\left(b^2(E - E_{22} - E_{33})(8a^2b^2E_{22} + (3a^4 - 4a^2b^2 + b^4)E_{33})\right. \\ & + 2\left(4a^2(a^2-b^2)L_{21}^2 + 2ab\left(8a^4 - \frac{10}{3}a^2b^2 - b^4\right)L_{21}L_{31}\right. \\ & \left.\left. + b^2(15a^4 + 8a^2b^2 + b^4)L_{31}^2\right)\right),\end{aligned} \tag{5.35}$$

which is described in the variables E_{22}, E_{33}, L_{21}, L_{31} only. We may take those variables as local coordinates of the orbit space $S^5/S^1 \cong \mathbf{C}P^2$, since they are mutually independent and invariant under the ϕ_t.

Our next task is to find a critical point for $\overline{H}_4$ and to prove that the critical point is non-degenerate. A straightforward calculation shows that if the matrices

$$A = -b^2\begin{pmatrix} 16a^2b^2 & (a^2+b^2)(3a^2+b^2) \\ (a^2+b^2)(3a^2+b^2) & 2(a^2-b^2)(3a^2-b^2)\end{pmatrix}, \tag{5.36}$$

$$B = 4\begin{pmatrix} 4a^2(a^2-b^2) & \frac{2}{3}ab(3a^2+b^2)(4a^2-3b^2) \\ \frac{2}{3}ab(3a^2+b^2)(4a^2-3b^2) & b^2(3a^2+b^2)(5a^2+b^2)\end{pmatrix} \tag{5.37}$$

are both non-degenerate, a critical point $\overline{p}$ for $\overline{H}_4$ is given by

$$E_{22} = \frac{-b^4(a^2-b^2)(3a^2-b^2)(3a^4-12a^2b^2+b^4)}{\det A}E, \tag{5.38a}$$

$$E_{33} = \frac{8a^2b^6(3a^4-12a^2b^2+b^4)}{\det A}E, \tag{5.38b}$$

$$L_{21} = L_{31} = 0, \tag{5.38c}$$

and further that it is non-degenerate. In fact, the Hessian for $\overline{H}_4$ is given by

$$\operatorname{Hess}\overline{H}_4 = \frac{1}{16a^4(a^2+b^2)^4}\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \tag{5.39}$$

with respect to the coordinates $E_{22}, E_{33}, L_{21}, L_{31}$. Thus, we conclude that there exists a periodic solution in a neighbourhood of $\Pi^{-1}(\overline{p})$, where $\Pi : S^5 \to S^5/S^1$.

We are now interested in a question as to whether small vibrations give rise to finite rotations or not. If the three-body system makes vibrational motions only, it satisfies the condition that $\boldsymbol{\pi} = 0$, which is written out as (3.2). Since we are working with small vibrations, we may set

$$g = \mathrm{e}^{\varepsilon\xi}, \qquad q = q_0 + \varepsilon\eta, \qquad \xi \in so(3). \tag{5.40}$$

Then, equation (3.2) reduces, at the order $O(\varepsilon)$, to

$$\dot{\xi} = -\sum_\alpha \Lambda_\alpha(q_0)\dot{\eta}_\alpha. \tag{5.41}$$

Integrated with respect to time, this equation provides $\xi(t)$ as a periodic function, if $\eta(t)$, a solution to (5.13), is periodic. This means that no effective rotation is caused by periodic small vibrations in the approximation of order $O(\varepsilon)$.

We have already obtained a perturbed periodic solution by Moser's procedure, which is well approximated by $(q(t), p(t)) = (q_0 + \varepsilon\eta(t), \varepsilon\zeta(t))$ with a suitable initial state $(\eta(0), \zeta(0))$. With this periodic solution, we may take into account the higher order term which was ignored in (5.41):

$$g^{-1}\frac{\mathrm{d}g}{\mathrm{d}t} = -\varepsilon\sum_\alpha \Lambda_\alpha(q_0)\dot{\eta}_\alpha - \varepsilon^2\sum_{\alpha,\beta}\frac{\partial\Lambda_\alpha}{\partial q_\beta}(q_0)\eta_\beta\dot{\eta}_\alpha + O(\varepsilon^3). \tag{5.42}$$

For simplicity, we take the periodic solution as approximated by $q(t) = q_0 + \varepsilon M^{-1}\eta'(t)$ with

$$\eta'_1(t) = c_1\sin t, \qquad \eta'_2(t) = c_2\cos t, \qquad \eta'_3(t) = c_3\sin t. \tag{5.43}$$

Using these functions together with (5.10), we obtain, after integration,

$$\varepsilon\sum_{\alpha,\beta}\frac{\partial\Lambda_\alpha}{\partial q_\beta}(q_0)\int_0^{2n\pi}\eta_\beta\dot{\eta}_\alpha\,\mathrm{d}t = n\varepsilon\frac{2(a^2-b^2)}{a^2+b^2}c_1c_2\pi R(\boldsymbol{e}_2). \tag{5.44}$$

This shows that for a sufficiently large n, the quantity εn becomes of order $O(1)$, if $a \neq b$. In other words, if $a \neq b$, after a sufficiently large number of periods of a perturbed small vibration, the integration of (3.2) may result in a finite rotation. We note here that if $a = b$ and if $m_1 = m_2 = m_3$, three particles form an equilateral triangle. By using the approximation $q(t) = q_0 + \varepsilon\eta(t)$, the rotation angle caused by the periodic solution can be calculated. In fact, in view of the connection form which has the $R(\boldsymbol{e}_2)$-component only, we may set $g = \mathrm{e}^{\theta(t)R(\boldsymbol{e}_2)}$. Then, equation (3.2) reduces to

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = -\varepsilon\sum_\alpha \lambda_\alpha(q_0 + \varepsilon\eta(t))\frac{\mathrm{d}\eta_\alpha}{\mathrm{d}t}, \tag{5.45}$$

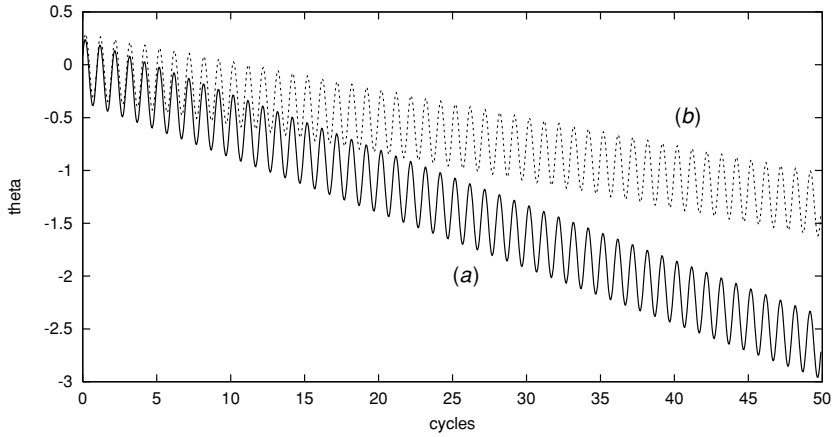

Figure 2. Rotation angle. Curve (a) shows the rotation angle derived by (5.45), while curve (b) is obtained by the integration of (5.42). A cycle means the period of a small vibration. The angle θ is measured with the unit of 10^{-2} rad.

where $\Lambda_\alpha(q) = \lambda_\alpha(q)R(\boldsymbol{e}_2)$. This equation is easily integrated to give a rotation angle, which can be interpreted as a contribution of the non-vanishing curvature (see (2.21)) on account of the Stokes theorem. An example of the numerical integration of the above equation is given in figure 2 with the graph of $\theta(t)$.

6. Linear triatomic molecules

We recall that the collinear configurations form the stratum M_1 which is the boundary of the principal stratum $\dot{M}$. To study boundary behaviour of a many-particle system in a neighbourhood of a collinear configuration in an explicit manner, we work with small vibrations of a linear triatomic molecule. The method of variational vectors on $\dot{M}/SO(3)$, which we explained in section 3, fails to apply. This is because the shape space $M_1/SO(3)$ for the collinear configurations of a triatomic molecule forms the boundary of the total shape space $M/SO(3)$. To see this, we recall that the projection $\pi : M \to M/SO(3)$ is realized by

$$w_1 = |\boldsymbol{r}_1|^2 - |\boldsymbol{r}_2|^2, \qquad w_2 = 2\boldsymbol{r}_1 \cdot \boldsymbol{r}_2, \qquad w_3 = 2|\boldsymbol{r}_1 \times \boldsymbol{r}_2|, \tag{6.1}$$

and that the whole shape space is homeomorphic with the closed half space [12, 13],

$$M/SO(3) \cong \{(w_1, w_2, w_3) \in \mathbf{R}^3 | w_3 \geqslant 0\}. \tag{6.2}$$

For collinear configurations, one has $w_3 = 0$, which determines the boundary plane, so that the tangent space to $M/SO(3)$ at a boundary point should be also homeomorphic with the closed half space. This prevents us from taking a variational 'vector' η at a boundary point.

Let $x_0 = (a\boldsymbol{e}_3, b\boldsymbol{e}_3) \in M_1, a > 0, b > 0$, be an equilibrium configuration. Rotational vectors at x_0 are given by

$$u_1 = R(\boldsymbol{e}_1)(a\boldsymbol{e}_3, b\boldsymbol{e}_3) = -(a\boldsymbol{e}_2, b\boldsymbol{e}_2), \tag{6.3a}$$

$$u_2 = R(\boldsymbol{e}_2)(a\boldsymbol{e}_3, b\boldsymbol{e}_3) = (a\boldsymbol{e}_1, b\boldsymbol{e}_1), \tag{6.3b}$$

which form an orthogonal basis of $V_{x_0} = T_{x_0}(\mathcal{O}_{x_0})$. Note that $R(\boldsymbol{e}_3)(a\boldsymbol{e}_3, b\boldsymbol{e}_3) = 0$. Vibrational vectors which are orthogonal to u_1, u_2 are given by

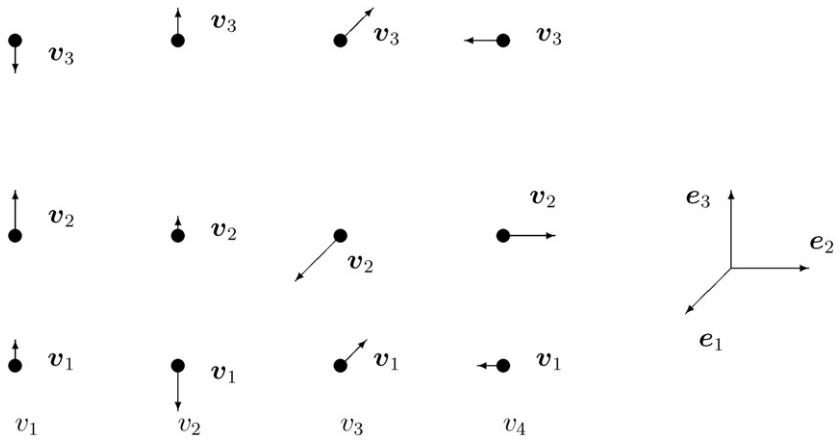

Figure 3. Vibrational vectors at a collinear configuration.

$$v_1 = (be_3, -ae_3), \tag{6.4a}$$

$$v_2 = (ae_3, be_3), \tag{6.4b}$$

$$v_3 = (be_1, -ae_1), \tag{6.4c}$$

$$v_4 = (be_2, -ae_2), \tag{6.4d}$$

which form an orthogonal basis of $H_{x_0} := V_{x_0}^{\perp}$. We have to note that v_1 and v_2 are tangent to M_1, but v_3 and v_4 are transversal to M_1. This means that v_1, v_2 and v_3, v_4 describe stretching and bending modes, respectively.

A question arises as to equations of motion for four modes. The bending motion brings a linear molecule into nonlinear configurations, and we have only three vibration modes for nonlinear configurations. How can one obtain equations of motion for a linear molecule with four vibration modes?

We recall here that the position vectors $(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$ and the Jacobi vectors $(\boldsymbol{r}_1, \boldsymbol{r}_2)$ are related by (5.1) and that the tangent vectors $(\dot{\boldsymbol{x}}_1, \dot{\boldsymbol{x}}_2, \dot{\boldsymbol{x}}_3)$ and $(\dot{\boldsymbol{r}}_1, \dot{\boldsymbol{r}}_2)$ are related likewise. For the vibrational vectors v_j, $j = 1, 2, 3, 4$, the component tangent vectors $(\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3)$ at respective particles can be described like (5.5). Since it is easy to find them, we do not write them, but give their figures only in figure 3.

The vectors v_j, $j = 1, \ldots, 4$, give rise to small displacements of the Jacobi vectors at the collinear configuration $x_0 = (ae_3, be_3)$;

$$(\delta \boldsymbol{r}_1, \delta \boldsymbol{r}_2) = \varepsilon \sum_{j=1}^{4} \eta_j' v_j, \tag{6.5}$$

where ε is an infinitesimal parameter, and η_j', $j = 1, \ldots, 4$, denote the Cartesian coordinates in H_{x_0}. From the definition of v_j, the $\delta \boldsymbol{r}_1$ and $\delta \boldsymbol{r}_2$ are expressed as

$$\delta \boldsymbol{r}_1 = \varepsilon((b\eta_1' + a\eta_2')\boldsymbol{e}_3 + b\eta_3'\boldsymbol{e}_1 + b\eta_4'\boldsymbol{e}_2), \tag{6.6a}$$

$$\delta \boldsymbol{r}_2 = \varepsilon((-a\eta_1' + b\eta_2')\boldsymbol{e}_3 - a\eta_3'\boldsymbol{e}_1 - a\eta_4'\boldsymbol{e}_2). \tag{6.6b}$$

Though the isotropy subgroup $\mathrm{e}^{tR(e_3)}$ at x_0 leaves x_0 fixed, it has a non-trivial action on the tangent space $T_{x_0}(M)$. In particular, it acts on the subspace H_{x_0} as follows:

$$e^{tR(e_3)}v_1 = v_1, \tag{6.7a}$$

$$e^{tR(e_3)}v_2 = v_2, \tag{6.7b}$$

$$e^{tR(e_3)}v_3 = v_3\cos t + v_4\sin t, \tag{6.7c}$$

$$e^{tR(e_3)}v_4 = -v_3\sin t + v_4\cos t. \tag{6.7d}$$

This implies that the vibration modes v_3 and v_4 are identical with each other in the sense that one of them may be realized by rotating the other one under the action of $e^{tR(e_3)}$. This implies that three modes, say, v_1, v_2, v_3, suffice for describing independent small vibrations in a small neighbourhood of $x_0 = (ae_3, be_3)$.

In the same manner as that for nonlinear molecules, we can express the small increments $\delta q_\alpha, \alpha = 1, 2, 3$, in terms of η'_α. We treat the collinear configurations as the limit of nonlinear configurations as $q_3 \to 0$ (see (4.6)). From the first two equations of (5.9) with $(q_1, q_2, q_3) = (a, b, 0)$, we obtain

$$\delta q_1 = \varepsilon(b\eta'_1 + a\eta'_2), \qquad \delta q_2 = \varepsilon(-a\eta'_1 + b\eta'_2). \tag{6.8}$$

To express δq_3, we need a limiting procedure. The third equation of (5.9) is differentiated to give

$$q_1q_3\delta q_1 + q_1^2\delta q_3 = (\delta r_1 \times r_2 + r_1 \times \delta r_2)\cdot\frac{r_1 \times r_2}{|r_1 \times r_2|}|r_1|. \tag{6.9}$$

We wish to make q_3 tend to zero in this equation. Since we work with vibrations, the total angular momentum vanishes, $r_1 \times \dot r_1 + r_2 \times \dot r_2 = 0$, and hence we obtain $(r_1 \times r_2)\cdot\dot r_1 = (r_1 \times r_2)\cdot\dot r_2 = 0$, which implies that vibrations take place in a constant plane [13]. This fact has been known in celestial mechanics [14]. On account of the symmetry around the e_3-axis of the collinear configuration, we may choose the plane of vibration to be the one spanned by e_3 and e_1, and set

$$r_1 \times r_2 = q_1q_3e_2. \tag{6.10}$$

Owing to this equation, we are allowed to take

$$\frac{r_1 \times r_2}{|r_1 \times r_2|}|r_1| \longrightarrow ae_2 \qquad \text{if} \quad (q_1, q_2, q_3) \to (a, b, 0). \tag{6.11}$$

Hence, equations (6.6), (6.9) and (6.11) are put together to give, as $(q_1, q_2, q_3) \to (a, b, 0)$,

$$\delta q_3 = -\varepsilon\left(\frac{a^2 + b^2}{a}\right)\eta'_3. \tag{6.12}$$

Introducing η_α by setting $\delta q_\alpha = \varepsilon\eta_\alpha, \alpha = 1, 2, 3$, we obtain

$$\eta_1 = b\eta'_1 + a\eta'_2, \tag{6.13a}$$

$$\eta_2 = -a\eta'_1 + b\eta'_2, \tag{6.13b}$$

$$\eta_3 = -\frac{a^2 + b^2}{a}\eta'_3. \tag{6.13c}$$

We have to make a remark on the range of η_3. In order that the limiting procedure be valid in the shape space, η should be taken as a tangent vector to $M/SO(3)$ at $q_0 \in M_1/SO(3)$. However, the tangent space $T_{q_0}(M/SO(3))$ as well as the shape space $M/SO(3)$ are topologically the closed half space (see (6.2)). Hence, the range of η_3 should be restricted to $\eta_3 \geqslant 0$ (see (5.9)), but η'_3 is not restricted. To make (6.13) valid for η_3 unrestricted, we have to extend the tangent space $T_{q_0}(M/SO(3))$. To this end, we make another projection

$(\boldsymbol{r}_1, \boldsymbol{r}_2) \mapsto (w_1, w_2, -w_3)$ to form a copy of the shape space, and piece it together with the original one along the boundary plane. We then obtain a doubled shape space which is homeomorphic with the whole space $\mathbf{R}^3$. Thus, we are allowed to extend the tangent space $T_{q_0}(M/SO(3))$ to be homeomorphic with $\mathbf{R}^3$. If this procedure is taken into account, equation (6.13) is regarded as a transformation rule in the extended tangent space $\widetilde{T}_{q_0}(M/SO(3))$ or in a doubled neighbourhood of q_0.

We now turn to the equation of small vibration. From (4.10), the metric tensor $(a_{\alpha\beta})$ at the point $(q_1, q_2, q_3) = (a, b, 0)$ is given by

$$G = (a_{\alpha\beta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{a^2}{a^2+b^2} \end{pmatrix}. \tag{6.14}$$

Let $M := \left(\frac{\partial \eta'_\alpha}{\partial \eta_\lambda}\right), \alpha, \lambda = 1, 2, 3$ along with (6.13). Then, the metric tensors, G and G', evaluated at $(q_1, q_2, q_3) = (a, b, 0)$ with respect to the coordinates (η_α) and (η'_α) are related by $G = M^T G' M$, so that one obtains

$$G'^{-1} = \frac{1}{a^2 + b^2} I, \tag{6.15}$$

where I is the 3×3 unit matrix.

Since v'_α given in (6.4) are orthogonal, we might think of the potential function for small vibrations as being given in H_{x_0} by

$$\tfrac{1}{2}\left(\kappa_1^2(\eta'_1)^2 + \kappa_2^2(\eta'_2)^2 + \kappa_3^2((\eta'_3)^2 + (\eta'_4)^2)\right). \tag{6.16}$$

However, on account of the fact that the plane of the small vibration is constant and of the $\mathrm{e}^{tR(\boldsymbol{e}_3)}$-symmetry, we should regard the potential function as being given by

$$V' = \tfrac{1}{2}\left(\kappa_1^2(\eta'_1)^2 + \kappa_2^2(\eta'_2)^2 + \kappa_3^2(\eta'_3)^2\right), \tag{6.17}$$

which projects to a function on a neighbourhood of $q_0 = \pi(x_0)$. We have to note that $\eta'_\alpha, \alpha = 1, 2, 3$, are viewed as local coordinates in a neighbourhood of q_0, if the extension of the shape space is taken into account.

We may now make $q_3 \to 0$ in the equation of small vibration (3.4) for a nonlinear molecule to obtain the equation of small vibration in a neighbourhood of a collinear shape. The resulting equation of small vibration for a linear molecule is put in the same form as (5.13)

$$\frac{\mathrm{d}^2\eta}{\mathrm{d}t^2} = -G^{-1}W\eta, \qquad W := \left(\frac{\partial^2 V}{\partial\eta_\alpha \partial\eta_\beta}\right), \qquad \alpha, \beta = 1, 2, 3, \tag{6.18}$$

but G and W are a bit different from those in (5.13); G is given by (6.14) and W results from (6.17) along with $\eta' = M\eta$. Equation (6.18) is diagonalized in terms of $\eta' = M\eta$. The equation of small vibration for η'_4 is the same as that for η'_3 because of the $\mathrm{e}^{tR(\boldsymbol{e}_3)}$-symmetry, where η'_4 is regarded as a coordinate in H_{x_0}.

Now we are interested in rotations caused by small vibrations. In what follows, we consider that the extension of the shape space is already performed and the extended cotangent space is denoted by $\widetilde{T}^*_{q_0}(M/SO(3))$ at the boundary point $q_0 \in M_1/SO(3)$. Now, we are to find a periodic solution, following Moser's averaging procedure. Since G'^{-1} and W' for a linear molecule are of the same form as those for a nonlinear molecule, the S^1 action determined by the small vibration is given by the same equation as (5.20). In the case of a linear molecule, the local coordinates in question are given by

$$(q_1, q_2, q_3) = (a, b, 0) + \varepsilon(\eta_1, \eta_2, \eta_3), \qquad (p_1, p_2.p_3) = \varepsilon(\zeta_1, \zeta_2, \zeta_3), \tag{6.19}$$

which is a bit different from (5.21). The (η, ζ) and (η', ζ') are related by

$$\eta' = M\eta, \qquad \zeta' = (M^T)^{-1}\zeta, \qquad M = \frac{1}{a^2+b^2}\begin{pmatrix} b & -a & 0 \\ a & b & 0 \\ 0 & 0 & -a \end{pmatrix}. \tag{6.20}$$

We take the potential function V as the same as (6.17). Like (5.23), the Hamiltonian is expanded into $\varepsilon^{-2}H = H_2 + \varepsilon H_3 + \varepsilon^2 H_4 + \cdots$, where

$$H_2 = \frac{1}{2}\left((a^2+b^2)\sum_\alpha \eta_\alpha'^2 + \frac{1}{a^2+b^2}\sum_\alpha \zeta_\alpha'^2\right), \tag{6.21}$$

$$H_3 = \frac{b}{a^2(a^2+b^2)}\big(-a\eta_1'\zeta_3'^2 + \eta_3'(a\zeta_1' - b\zeta_2')\zeta_3'\big), \tag{6.22}$$

$$H_4 = \frac{1}{2a^4(a^2+b^2)}\big((a^2+b^2)^2\eta_3'^2(a\zeta_1' - b\zeta_2')^2 \tag{6.23}$$

$$- a((a^2+2b^2)\eta_1' + ab\eta_2')\eta_3'(a\zeta_1' - b\zeta_2')\zeta_3' + a^2\eta_1'((a^2+3b^2)\eta_1' + 2ab\eta_2')\zeta_3'^2\big). \tag{6.24}$$

The averages of H_2 and of H_1 are the same as (5.30). The average of H_4 is given by

$$\overline{H}_4 = \frac{1}{16a^4(a^2+b^2)}\big((a^2(a^2+2b^2)E_{11} + b^2(2a^2+b^2)E_{22})E_{33} + 2\big(3a^4(a^2+2b^2)L_{31}^2 - 4ab^3L_{31}L_{32} + b^4L_{32}^2\big)\big). \tag{6.25}$$

We may take E_{11}, E_{22}, L_{31}, L_{32} as local coordinates in the orbit space. It then follows that if the matrices

$$A = -\begin{pmatrix} 2a^2(a^2+2b^2) & a^4+4a^2b^2+b^4 \\ a^4+4a^2b^2+b^4 & 2b^2(2a^2+b^2) \end{pmatrix}, \tag{6.26}$$

$$B = 4\begin{pmatrix} 3a^2(a^2+2b^2) & -2ab^3 \\ -2ab^3 & b^4 \end{pmatrix} \tag{6.27}$$

are both non-degenerate, a critical point $\overline{p}$ of $\overline{H}_4$ is given by

$$E_{11} = \frac{-b^2(2a^2+b^2)}{(a^2+b^2)(a^2-b^2)}E, \tag{6.28a}$$

$$E_{22} = \frac{a^2(a^2+2b^2)}{(a^2+b^2)(a^2-b^2)}E, \tag{6.28b}$$

$$L_{31} = L_{32} = 0, \tag{6.28c}$$

and it is non-degenerate on account of

$$\operatorname{Hess}\overline{H}_4 = \frac{1}{16a^4(a^2+b^2)}\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}. \tag{6.29}$$

Thus, there exists a periodic solution $(q(t), p(t))$ in a neighbourhood of $\Pi^{-1}(\overline{p})$, where $\Pi : S^5 \to S^5/S^1$.

As was pointed out already in section 4, the matrix functions $\Lambda_\alpha(q)$ remain to be defined if $q_3 \to 0$. Then we may deal with equation (3.2) in the limit as $q_3 \to 0$. It then turns out that, like nonlinear molecules, no effective rotation is caused by small vibrations at the order

$O(\varepsilon)$. We turn to the expansion (5.42) with the periodic solution $(q(t), p(t))$ found above. We assume here that the $q(t)$ is approximated by $q(t) = q_0 + \varepsilon M^{-1}\eta'(t)$ with

$$\eta_1'(t) = c_1 \sin t, \qquad \eta_2'(t) = c_2 \sin t, \qquad \eta_3'(t) = c_3 \cos t. \tag{6.30}$$

Then, after a straightforward calculation, we obtain

$$\varepsilon \sum_{\alpha,\beta=1}^{3} \frac{\partial \Lambda_\alpha}{\partial q_\beta}(q_0) \int_0^{2n\pi} \eta_\beta \dot{\eta}_\alpha \, \mathrm{d}t = -2n\varepsilon c_1 c_3 \pi R(\boldsymbol{e}_2). \tag{6.31}$$

From this, we observe that the quantity εn becomes of order $O(1)$ for a sufficiently large n. This implies that after a sufficiently large number of periods of the perturbed small vibration the linear molecule may get rotated by an finite angle.

7. Remarks on boundary behaviour

In this section, we make some remarks on boundary behaviour in the shape space for the three-body system. We first consider a geodesic passing $x_0 = (a\boldsymbol{e}_3, b\boldsymbol{e}_3) \in M_1$ at $t = 0$, which is expressed as $x(t) = x_0 + \sum_{j=0}^{4} v_j c_j t$ or

$$\boldsymbol{r}_1(t) = bc_3 t\boldsymbol{e}_1 + bc_4 t\boldsymbol{e}_2 + (a + (bc_1 + ac_2)t)\boldsymbol{e}_3, \tag{7.1a}$$

$$\boldsymbol{r}_2(t) = -ac_3 t\boldsymbol{e}_1 - ac_4 t\boldsymbol{e}_2 + (b + (-ac_1 + bc_2)t)\boldsymbol{e}_3. \tag{7.1b}$$

The line $x(t)$ is horizontal, since $\boldsymbol{r}_1(t) \times \dot{\boldsymbol{r}}_1(t) + \boldsymbol{r}_2(t) \times \dot{\boldsymbol{r}}_2(t) = 0$, as is verified easily. We now calculate the vector product $\boldsymbol{r}_1 \times \boldsymbol{r}_2$ to obtain

$$w_3(t) = 2|\boldsymbol{r}_1 \times \boldsymbol{r}_2| = 2(a^2 + b^2)\sqrt{c_3^2 + c_4^2}|t(1 + c_2 t)|, \tag{7.2}$$

which vanishes at $t = 0$ and $t = -1/c_2$. This means that the projected curve $w(t) = \pi(x(t))$ with $t \neq 0, t \neq -1/c_2$, which is a geodesic in $\dot{M}/SO(3)$ with respect to the metric $(a_{\alpha\beta})$, reaches boundary points of the whole shape space $M/SO(3)$ when $t = 0$ and $t = -1/c_2$. Hence, the Riemannian manifold $\dot{M}/SO(3)$ is not geodesically complete. The geodesic $w(t)$ bounces on the boundary plane. The one-sided tangent vector to $w(t)$ at $t = 0$ is easy to calculate:

$$\dot{w}_j(-0) = \dot{w}_j(+0), \qquad j = 1, 2, \qquad -\dot{w}_3(-0) = \dot{w}_3(+0). \tag{7.3}$$

The same equations are obtained for $t = -1/c_2$. Thus, we observe that the one-sided tangent vectors $\dot{w}(+0)$ and $\dot{w}\left(-\frac{1}{c_2} + 0\right)$ are the reflections of $\dot{w}(-0)$ and of $\dot{w}\left(-\frac{1}{c_2} - 0\right)$, respectively. In the doubled shape space (stated in section 6), the geodesic $w(t)$ passes the boundary to get into the region of $w_3 < 0$.

We turn to a small vibration given by $x(t) = x_0 + \sum_{j=1}^{4} \eta_j'(t)v_j$ for a linear molecule, which projects through (6.1) to a curve in the shape space:

$$\begin{aligned} w_1(t) = {} & (b^2 - a^2)(\eta_1'(t)^2 - \eta_2'(t)^2 + \eta_3'(t)^2 + \eta_4'(t)^2) + 4ab\eta_1'(t)\eta_2'(t) \\ & + 4ab\eta_1'(t) + 2(a^2 - b^2)\eta_2'(t) + a^2 - b^2, \end{aligned} \tag{7.4a}$$

$$\begin{aligned} w_2(t) = {} & -2ab(\eta_1'(t)^2 - \eta_2'(t)^2 + \eta_3'(t)^2 + \eta_4'(t)^2) + 2(b^2 - a^2)\eta_1'(t)\eta_2'(t) \\ & + 2(b^2 - a^2)\eta_1'(t) + 4ab\eta_2'(t) + 2ab, \end{aligned} \tag{7.4b}$$

$$w_3(t) = 2(a^2 + b^2)|1 + \eta_2'(t)|\sqrt{\eta_3'(t)^2 + \eta_4'(t)^2}. \tag{7.4c}$$

These equations show that a small vibration projects to an oscillation bouncing on the boundary plane $w_3 = 0$. If we take the doubled shape space into account, the projection $w(t)$ becomes an

oscillation passing the boundary with sgn w_3 alternating. From (7.4), we observe further that small vibrations which have the same $\eta_3'(t)^2 + \eta_4'(t)^2$ project to the same curve $\pi(x(t))$ in the shape space. In particular, small vibrations $x(t) = x_0 + \eta_3'(t)v_3$ and $y(t) = x_0 + \eta_4'(t)v_4$ with $|\eta_3'(t)| = |\eta_4'(t)|$ share the same projection in the shape space. This implies that the bending modes, v_3 and v_4, related by the symmetry $\mathrm{e}^{tR(e_3)}$ are not distinguishable, when projected on the shape space.

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