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Classical "Freezing" of Plane Rotations: A Proof of the Boltzmann–Jeans Conjecture

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Using simple known methods and results of classical perturbation theory, especially those due to Nekhoroshev and Neishtadt, we study the energy exchanges between the rotational and the translational degrees of freedom in a particular model representing the planar motion of a rigid body in a bounded analytic potential. We prove that, if the angular velocity ω is initially large, then the energy exchanges are small, $\mathcal{O}(\omega^{-1})$, for times growing exponentially with ω, $|t| \sim \exp \omega$. We also deduce that in a scattering process from a (smooth) potential barrier, the overall change in the rotational energy of the incoming body is exponentially small in ω, $\mathcal{E} \sim \exp(-\omega)$. The results are interpreted in the light of an old conjecture by Boltzmann and Jeans on the existence of very large time scales for equilibrium in statistical systems containing high-frequency degrees of freedom (purely classical "freezing" of the high-frequency degrees of freedom); the rotating object is, in this interpretation, a (classical) molecule, which moves in an external field, or collides with the wall of a container. Two different limits of large ω are considered, namely the limit of large rotational energy, and (as is interesting for the molecular interpretation) the limit of point mass, at finite rotational energy.

KEY WORDS: Perturbation theory; exponential estimates; equipartition rate; Boltzmann–Jeans conjecture.

1. INTRODUCTION

1.1. This paper is devoted to a study of the planar motion of a fast rotating rigid body, in the realm of Hamiltonian perturbation theory. Denoting by $q = (q_1, q_2)$ the coordinates of the center of mass, by φ an

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angle giving the orientation of the body, and by $p=(p_1, p_2)$ and I the corresponding momenta, the Hamiltonian has the form

$$h(p, q, I, \varphi)=\frac{I^2}{2C}+\frac{p^2}{2m}+v(q, \varphi) \tag{1.1}$$

where $q\in\mathbb{R}^2$, $p\in\mathbb{R}^2$, $I\in\mathbb{R}$, $\varphi\in S^1$, and $p^2=p_1^2+p_2^2$; the constants m and C denote, respectively, the mass and the moment of inertia of the body. The purely positional potential v is assumed to be real analytic and bounded.

Because of the coupling term v, there could be in principle any transfer of energy between the rotational and the translational degrees of freedom. Nevertheless, using ideas and adapting results of perturbation theory, due essentially to Nekhoroshev[1-3] and Neishtadt,[4] we show that, if the angular velocity $\omega(I)=I/C$ is initially large, then significant energy exchanges can take place only on extremely long time scales. Indeed, it turns out that the energy exchanges remain small, say $\mathcal{O}(\omega^{-1})$, for a time scale $\mathcal{T}$ growing exponentially fast with ω:

$$\mathcal{T}=\mathcal{T}_0\exp(\tau\omega) \tag{1.2}$$

$\mathcal{T}_0$ and τ are suitable constants.

Moreover, we consider explicitly the case of the scattering of the body by a fixed obstacle; we describe the obstacle by a smooth potential, decaying at infinity in an integrable way, and prove that after the scattering, the rotational energy $I^2/2C$ differs from the initial value by a quantity $\mathcal{E}$ exponentially small with ω,

$$\mathcal{E}=\mathcal{E}_0\exp(-\tau\omega) \tag{1.3}$$

One should remark that the angular velocity ω of the body can be large either because I is large (limit of high rotational energy), or else, at fixed finite rotational energy, because C is small (limit of point mass). The latter is the case of a small body of diameter proportional to a small parameter ε. The moment of inertia is then $C=\mathcal{O}(\varepsilon^2)$, so that for small values of the angular momentum, $I=\mathcal{O}(\varepsilon)$, one has $\omega=\mathcal{O}(\varepsilon^{-1})$ and $I^2/2C=\mathcal{O}(1)$. We shall consider both these cases.

1.2. Apart from the (strong) limitation to two dimensions (see the Conclusions for comments), such problems arise in quite different frameworks: for instance, the body could be a fast rotating nonspherical asteroid having a close encounter with a planet. However, our personal motivations come from microphysics, namely from an old, almost forgotten conjecture by Boltzmann[5] and Jeans,[6,7] only recently reconsidered (see refs. 8–12). The essence of this conjecture (which was proposed before the advent of quantum mechanics) is that the "freezing" of the high-frequency degrees of freedom (today often reported as a typical purely quantum feature) could be explained classically, as a nonequilibrium phenomenon.

Let us consider, as a model example, a diatomic gas. On the basis of the principle of equipartition of energy, one expects (classically) seven contributions per molecule to the specific heat (three from translations, two from rotations, one kinetic and one potential from vibrations), so that $C_v = \frac{7}{2}R$. On the contrary, at ordinary temperatures one finds $C_v = \frac{5}{2}R$ (freezing of vibrations), and at lower temperatures, $C_v = \frac{3}{2}R$ (freezing of rotations), as for monoatomic gases. Moreover, following Boltzmann, in principle one should also take into consideration the internal degrees of freedom of the atoms, and thus expect a higher specific heat, even in the case of monoatomic gases; in fact, even if one represents an atom as a small hard sphere, neglecting any further internal structure, one should wonder, classically, why its rotational degrees of freedom do not contribute to the specific heat (actually, we study the point-mass limit just as a model for this question).

The answer proposed by Boltzmann and Jeans is simply that an appreciable energy exchange with a high-frequency degree of freedom requires an extremely long time scale ("years"[5]; "hundreds of centuries"[6]), so that, in any reasonable experiment, these degrees of freedom behave as if they were frozen. Jeans, in particular, on the basis of some heuristic considerations, proposed an exponential law for the energy exchange due to a collision which is precisely of the form (1.3) and, correspondingly, a relaxation time growing exponentially with ω, as in (1.2). A similar law was later reconsidered, in a different framework, by Landau and Teller,[13] still on the basis of heuristic considerations; it also appears in connection with collisions of molecules (see typically ref. 14) or in plasma physics (see, for example, ref. 15). None of these authors, however, is apparently aware of Jeans' ideas.

The conjecture by Boltzmann and Jeans was successfully tested numerically[8] on an oversimplified one-dimensional model of purely vibrating and translating molecules. The freezing of fast vibrations was later proven analytically, within suitable assumptions, in refs. 9 and 10. Concerning the freezing of fast rotations, in the case of high rotational energy, an accurate numerical study for a planar model of the form (1.1) is reported in ref. 16, which is rather deeply connected to the present paper.[3] In this paper, we perform a further step toward the understanding

[3] Strong evidence is given there of the possible "freezing" of the rotational degrees of freedom for macroscopic times.

of the Boltzmann–Jeans conjecture, by providing the analytical proof of the exponential laws (1.2) and (1.3) for a Hamiltonian like (1.1).

1.3. A natural tool for problems with fast and slow variables is classical perturbation theory. As a matter of fact, the proofs we are looking for are rather simple applications of the ideas and techniques of the Nekhoroshev theorem[1–3] (see also refs. 17 and 18). More specifically, our results for the case of large rotational energy ($\omega \to \infty$ at fixed moment of inertia) are in principle contained in a paper by Neishtadt.[4] Unfortunately, the theorem proved by Neishtadt is too general, and not sufficiently detailed, for our purposes; in addition, no explicit estimate of the relevant constants is there produced. We reconsider Neishtadt's results here. Let us also remark that the point-mass limit ($I^2/2C$ fixed, $C \to 0$) cannot be deduced from the previous case by a simple rescaling. Indeed, in order to keep finite the rotational energy, one must take $I = \mathcal{O}(\varepsilon)$; one is then forced to use a perturbative scheme in which the I domain shrinks to zero for $\varepsilon \to 0$, and consequently the whole perturbation scheme gets modified (in fact, such a case resembles more closely the one of refs. 9, 10, and 19 rather than the Neishtadt one). For brevity, we shall not give complete proofs for this case, limiting ourselves to a sketch of the differences.

1.4. The paper is organized as follows. Section 2 and 3 are devoted to the case of high rotational energy; in Section 2 we appropriately formulate the problem, and state a basic proposition (Proposition 1), while in Section 3 we deduce from it two corollaries, concerning the exponential laws (1.2) and (1.3). Section 4 is devoted to the point-mass limit. Section 5 reports the proof of Proposition 1, together with a sketch of the similar proof for the point-mass limit. A conclusion follows.

2. THE PERTURBATIVE APPROACH

Let us formulate the problem in a slightly more general and mathematically more suitable framework. We consider the Hamilton function

$$h(p, q, I, \varphi) = k(I) + u(p, q, I, \varphi) \tag{2.1}$$

and assume it be real analytic for $(p, q) = (p_1, \dots, p_n, q_1, \dots, q_n) \in \mathscr{B}$, a domain in $\mathbb{R}^{2n}$ ($n \geq 1$), $I \in \mathscr{I}$, a real interval (or just a point), and $\varphi \in S^1$. In the sequel, we shall denote $z = (p, q, I)$ and let

$$\Delta_0 = \mathscr{B} \times \mathscr{I}, \qquad \mathscr{D}_0 = \Delta_0 \times S^1$$

[so that $z \in \Delta_0$ and $(z, \varphi) \in \mathscr{D}_0$]. We shall assume that the Hamiltonian (2.1) has an analytic extension, bounded together with its first derivatives, to a complex neighborhood $\mathscr{D}_\rho$ of $\mathscr{D}_0$, defined as follows. With reference to an "extension vector"

$$\rho = (\rho_p, \rho_q, \rho_I, \rho_\varphi) \tag{2.2}$$

having positive entries (which will play the role of parameters), we introduce the polydisc $\Delta_{\rho,z}$, the strip $\mathscr{S}_\rho$, and the domain Δ_ρ defined by

$$\Delta_{\rho,z} = \{z' \in \mathbb{C}^{2n+1}: |I' - I| < \rho_I, |p'_j - p_j| < \rho_p, |q'_j - q_j| < \rho_q, j = 1,..., n\}$$
$$\mathscr{S}_\rho = \{\varphi \in \mathbb{C}: |\mathrm{Im}\ \varphi| < \rho_\varphi\}$$
$$\Delta_\rho = \bigcup_{z \in \Delta_0} \Delta_{\rho,z}$$

We then consider the complex domains

$$\mathscr{D}_\rho = \Delta_\rho \times \mathscr{S}_\rho, \qquad \mathscr{D}_{\rho,z} = \Delta_{\rho,z} \times \mathscr{S}_\rho \quad (z \in \Delta_0) \tag{2.3}$$

Notice that the latter is global in the angle φ, but local in the remaining coordinates. These local domains are important only for the case of the scattering.

Inequalities of the form $\rho' < \rho$, for extension vectors, are intended to work separately on each entry; with no possibility of confusion, we shall denote by ρ both the vector in (2.2) and the real number ρ defined by

$$\rho^2 = \min(\rho_p \rho_q, \rho_I \rho_\varphi) \tag{2.4}$$

For practical convenience, the nonrestrictive assumption $\rho_\varphi \leqslant 1$ is made.

Concerning norms, we refer to the supremum norm, and denote, for any function $w: \mathscr{D}_\rho \to \mathbb{C}$,

$$|w|_\rho = \sup_{(z,\varphi) \in \mathscr{D}_\rho} |w(z, \varphi)| \tag{2.5}$$

The use of the "local norm"

$$|w|_{\rho,z} = \sup_{(z',\varphi) \in \mathscr{D}_{\rho,z}} |w(z', \varphi)|, \qquad z \in \Delta_0 \tag{2.6}$$

will be relevant for the treatment of the scattering. We shall also consider a "vector field norm" of functions, defined in the following way: for any vector $\sigma \leqslant \rho$, and any function $w: \mathscr{D}_\sigma \to \mathbb{C}$, we let

$$\|w\|_\sigma = \max_{a = p,q,I,\varphi} \rho_a \left|\frac{\partial w}{\partial a}\right|_\sigma \tag{2.7}$$

Clearly, this is nothing but a convenient norm of the Hamiltonian vector field W corresponding to the Hamilton function w, namely, with obvious notation,

$$W = -\frac{\partial w}{\partial q}\partial_p + \frac{\partial w}{\partial p}\partial_q - \frac{\partial w}{\partial \varphi}\partial_I + \frac{\partial w}{\partial I}\partial_\varphi \tag{2.8}$$

One could remark that one does not really need to introduce such a norm (indeed, it would be enough to assume that w is analytic in $\mathscr{D}_{2\rho}$ to have, by Cauchy inequality, $\|w\|_\rho \leqslant |w|_{2\rho}$). Nevertheless, it is in a sense more natural, and perhaps illuminating, to distinguish, in the statements as well in the proofs, between properties intrinsically connected to the norm of the Hamilton functions (essentially, properties related to the energy conservation) and properties that are instead more directly related to the norm of the corresponding vector fields.

The natural small parameter of the perturbative treatment will be Ω_0/Ω, where

$$\Omega = \inf_{I \in \mathscr{D}_\rho} \left| \frac{\partial k}{\partial I}(I) \right|, \qquad \Omega_0 = \rho^{-2} \|u\|_\rho \tag{2.9}$$

The interpretation of Ω_0 is easy: its inverse gives, in the simplest (perhaps not optimal) way, a time scale naturally associated to u in the Hamiltonian (2.1). The constant

$$C^{-1} = \left| \frac{\partial^2 k}{\partial I^2} \right|_\rho \tag{2.10}$$

will also have some role [C is the moment of inertia, if $k(I)$ is quadratic in I].

Working perturbatively, we give the Hamiltonian (2.1) a φ-independent normal form, up to a remainder exponentially small in Ω. Precisely, we prove the following Proposition:

Proposition 1. Within the above notations and assumptions, let

$$\Omega \geqslant \max\left(\Omega^*, \frac{8\rho_I}{C\rho_\varphi}\right) \tag{2.11}$$

where

$$\Omega^* = 2^{10}\Omega_0 = \frac{2^{10}}{\rho^2}\|u\|_\rho \tag{2.12}$$

Then: (i) one can construct a real analytic canonical transformation $\mathscr{C}: \mathscr{D}_{\frac{1}{2}\rho} \to \mathscr{D}_\rho$, $(z, \varphi) = \mathscr{C}(z', \varphi')$, which gives the new Hamiltonian $h' = h \circ \mathscr{C}$ the form

$$h' = k(I') + \bar{u}(p', q', I') + \frac{\Omega^*}{\Omega} g(p', q', I') + \frac{\Omega^*}{\Omega} e^{-[\Omega/\Omega^*]} f(p', q', I', \varphi') \tag{2.13}$$

where $[\cdot]$ denotes the integer part, and $\bar{u} = (2\pi)^{-1} \int_0^{2\pi} u \, d\varphi$ is the average of u on φ.

(ii) For any $z \in \Delta_0$, the functions g and f in (2.13) satisfy the (local) estimates

$$|g|_{\frac{1}{2}\rho, z} \leqslant 2^{-3} |u - \bar{u}|_{\rho, z} \tag{2.14a}$$

$$|f|_{\frac{1}{2}\rho, z} \leqslant 2^{-5} |u - \bar{u}|_{\rho, z} \tag{2.14b}$$

$$\left| \frac{\partial f}{\partial \varphi} \right|_{\frac{1}{2}\rho, z} \leqslant 2^{-2} \left| \frac{\partial u}{\partial \varphi} \right|_{\rho, z} \tag{2.14c}$$

(iii) The diffeomorphism $\mathscr{C}$ is close to the identity: precisely, for any $(z, \varphi) \in \mathscr{D}_{\frac{1}{2}\rho}$ and any function $w: \mathscr{D}_\rho \to \mathbb{C}$, one has

$$|a' - a| \leqslant \frac{16}{\Omega} \left| \frac{\partial u}{\partial \bar{a}} \right|_{\rho, z} \leqslant 2^{-6} \frac{\Omega^*}{\Omega} \rho_a \qquad (a = p, q, I) \tag{2.15a}$$

$$|\varphi' - \varphi| \leqslant \frac{16}{\Omega \rho_I} \|u\|_{\rho, z} \leqslant 2^{-6} \frac{\Omega^*}{\Omega} \rho_\varphi \tag{2.15b}$$

$$|w(z', \varphi') - w(z, \varphi)| \leqslant 2^{-3} \frac{\Omega^*}{\Omega} |w|_{\rho, z} \tag{2.15c}$$

where $\bar{a}$ denotes the variable conjugate to a.

The proof of Proposition 1 is deferred to Section 5.

3. FREEZING OF HIGH-ENERGY ROTATIONS

We consider here the particular case of the Hamiltonian (1.1), i.e., the case $n = 2$, $k = I^2/2C$, $u = p^2/2m + v(q, \varphi)$. We draw from Proposition 1 two corollaries, one relative to the general case of a bounded potential, the other dedicated to the special case of scattering.

3.1. Freezing of Fast Rotations

Let us write $h = \hat{h} + \tilde{h}$, with

$$\hat{h} = \frac{p^2}{2m} + \bar{v}(q), \qquad \tilde{h} = \frac{I^2}{2C} + v(q, \varphi) - \bar{v}(q) \tag{3.1}$$

Our aim is to show that, if the initial angular velocity $\omega = C^{-1} |I(0)|$ is large enough, then it changes little and, moreover, $\hat{h}$ and $\tilde{h}$ are separately almost constant, for times growing exponentially with ω.

To be definite, we assume that $v(q, \varphi)$ is everywhere bounded and, more precisely, that it has a bounded analytic extension to the set $\{(q, \varphi) \in \mathbb{C}^3\colon |\mathrm{Im}\, q_1| < \rho_q,\ |\mathrm{Im}\, q_2| < \rho_q,\ |\mathrm{Im}\, \varphi| < \rho_\varphi\}$, for some $\rho_q > 0$ and $\rho_\varphi > 0$.

Corollary 1. Within the above hypotheses, consider a positive number $E \geqslant 2(\|v\|_\rho + |v|_\rho)$, and let

$$\omega^* = \frac{2^{13}}{\rho_q} \left(\frac{2E}{m}\right)^{1/2} \tag{3.2}$$

Then, any real motion $(p(t), q(t), I(t), \varphi(t))$ of system (1.1) whose initial data are such that

$$\frac{p(0)^2}{2m} \leqslant E \tag{3.3a}$$

$$\omega = \frac{I(0)}{C} \geqslant \max\left(2\omega^*, \frac{16\rho_q}{C\rho_\varphi^2} (2mE)^{1/2}\right) \tag{3.3b}$$

satisfies[4]

$$|I(t) - I(0)| \leqslant \frac{2^6}{\omega} \left|\frac{\partial v}{\partial \varphi}\right|_\rho \tag{3.4a}$$

$$\left|\frac{I^2}{2C} + v - \bar{v}\right|_0^t \leqslant 3 \frac{\omega^*}{\omega} E \tag{3.4b}$$

for

$$|t| \leqslant \frac{2\rho_\varphi}{\omega} \exp\left[\frac{\omega}{\omega^*}\right] \tag{3.5}$$

[4] Here and in the following we use, for any function x, the short notation $|x|_0^t = |x(t) - x(0)|$.

Proof. We apply Proposition 1, with $\mathscr{B} = \{q \in \mathbb{R}^2,\ p^2/2m \leqslant E\}$, $\mathscr{I} = \{I(0)\}$, $\rho_p = 2(2mE)^{1/2}$, and $\rho_I = \rho_p \rho_q/\rho_\varphi$. An easy calculation then gives

$$\left|\frac{p^2}{2m}\right|_\rho = 9E, \qquad \left\|\frac{p^2}{2m}\right\|_\rho = 12E$$
$$\frac{\|u\|_\rho}{\rho^2} \leqslant \frac{3}{\rho_q}\left(\frac{2E}{m}\right)^{1/2}, \qquad \omega^* \geqslant 2\Omega^* \tag{3.6}$$

Furthermore, one has clearly $\Omega = \omega - \rho_I/C$, so that, by (3.3b) and (3.2), $\Omega \geqslant \omega/2$ and $\Omega/\Omega^* \geqslant \omega/\omega^*$.

Consider now a real motion $(z(t), \varphi(t))$, with $z(0) \in \Delta_0$, and let T_{esc} be its (possibly infinite) escape time from $\mathscr{D}_{\frac{1}{2}\rho}$. From (2.13) and (2.14) one derives

$$|I'(t) - I'(0)| \leqslant |t| \,\frac{1}{4}\frac{\omega^*}{\omega}\, e^{-[\omega/\omega^*]} \left|\frac{\partial v}{\partial \varphi}\right|_\rho \tag{3.7}$$

as long as $|t| \leqslant T_{\text{esc}}$, and consequently

$$|I'(t) - I'(0)| \leqslant \frac{1}{2}\frac{\omega^*}{\omega^2}\left|\frac{\partial v}{\partial \varphi}\right|_\rho \rho_\varphi \tag{3.8}$$

for $|t| \leqslant \min(T_{\text{esc}}, T)$, T being defined by the rhs of (3.5). From (3.8), (2.15a), (3.2), and (3.3b), one gets the two inequalities

$$|I(t) - I(0)| \leqslant \frac{1}{2}\frac{\omega^*}{\omega^2}\left|\frac{\partial v}{\partial \varphi}\right|_\rho \rho_\varphi + \frac{32}{\omega}\left|\frac{\partial v}{\partial \varphi}\right|_\rho < \frac{2^6}{\omega}\left|\frac{\partial v}{\partial \varphi}\right|_\rho \tag{3.9a}$$

$$|I(t) - I(0)| \leqslant \frac{1}{2}\frac{\omega^*}{\omega^2}\left|\frac{\partial v}{\partial \varphi}\right|_\rho \rho_\varphi + 2^{-6}\frac{\omega^*}{\omega}\rho_I < 2^{-5}\frac{\omega^*}{\omega}\rho_I \tag{3.9b}$$

the first of which proves (3.4a), for times $|t| \leqslant \min(T_{\text{esc}}, T)$.

Concerning (3.4b), one first computes, using again (3.8), (2.15a), and (3.3b),

$$\left|\frac{I'^2}{2C}\right|_0^t \leqslant \frac{1}{2C}\,|I'(t) - I'(0)|\,[\,|I'(t) - I'(0)| + 2\,|I'(0) - I(0)| + 2\,|I(0)|\,]$$
$$\leqslant 0.6\,\frac{\omega^*}{\omega}\,\|v\|_\rho$$

Thus, using energy conservation and then the inequalities (2.14a) and (2.14b), one gets

$$|\hat{h}(p', q')|_0^t \leqslant \left|\frac{I'^2}{2C}\right|_0^t + \frac{\omega^*}{\omega}\left(|g|_0^t + e^{-[\omega/\omega^*]}\,|f|_0^t\right) \leqslant \frac{1}{2}\frac{\omega^*}{\omega}E \tag{3.10}$$

Applying (2.15c) to the function $\hat{h}$, one then obtains

$$|\hat{h}(p, q)|_0^t \leqslant |\hat{h}(p', q')|_0^t + \frac{1}{4}\frac{\omega^*}{\omega}|\hat{h}|_\rho \leqslant 3\frac{\omega^*}{\omega}E \tag{3.11}$$

We now show that, under the stated hypotheses, $T_{\text{esc}} \geqslant T$. To this purpose, one needs to show that the coordinates $p(t)$ and $I(t)$ do not escape $\mathscr{D}_{\frac{1}{2}\rho}$, for $|t| \leqslant T$. This is seen by the standard argument: should one have $T_{\text{esc}} < T$, then at $t = T_{\text{esc}}$, one at least of (3.4) would be violated. For the latter coordinate, this is assured by (3.9b); on the other hand, in order for $p(t)$ to escape $\mathscr{D}_{\frac{1}{2}\rho}$, one would need $p(t)^2/2m > 4E$, and thus $|p(t)^2/2m - p(0)^2/2m| > 3E$, $|\hat{h}(t) - \hat{h}(0)| > 3E - 2|v|_\rho \geqslant 2E$, which is in conflict with (3.4b) if $\omega \geqslant 2\omega^*$. ∎

3.2. The Scattering

We come now to the scattering problem; here we shall use in an essential way the local estimates. First of all, we say that we have a "scattering trajectory" $(p(t), q(t), I(t), \varphi(t))$, $-\infty < t < +\infty$, if the following conditions are fulfilled:

$$\lim_{t \to \pm\infty} |q(t)| = \infty \tag{3.12a}$$

$$\lim_{t \to \pm\infty} p(t) = p^{\pm} \neq 0 \tag{3.12b}$$

$$\beta := \int_{-\infty}^{+\infty} \left|\frac{\partial v}{\partial \varphi}\right|_{\rho, z(t)} dt < \infty \tag{3.12c}$$

In particular, the latter condition assures that $(\partial v/\partial\varphi)(q(t), p(t))$ goes to zero sufficiently fast for $t \to \pm\infty$, so that the limits $I(\pm\infty)$ also exist. Of course, one could make assumptions on v (essentially, repulsivity with reference to a fixed scatterer) which ensure the existence of scattering trajectories: however, assuming directly (3.12) is simpler and, in our opinion, more natural in the present framework. The following corollary is then easily deduced:

Corollary 2. For any scattering trajectory, with p^- and $\omega = C^{-1}I(-\infty)$ satisfying the conditions (3.3), one has

$$\left|\frac{I(+\infty)^2}{2C} - \frac{I(-\infty)^2}{2C}\right| < \frac{1}{4}\beta\gamma\omega^* \exp - \left[\frac{\omega}{\omega^*}\right] \tag{3.13}$$

with

$$\gamma = 1 + \frac{\beta}{8\omega C} \frac{\omega^*}{\omega} e^{-[\omega/\omega^*]}$$

ω^* is given by (3.2).

Proof. One makes the same choice of domains and complex extensions as for the proof of Corollary 1. In addition to the conclusions of Corollary 1, one has now

$$|I'(+\infty) - I'(-\infty)| \leqslant \frac{1}{4} \frac{\omega^*}{\omega} e^{-[\omega/\omega^*]} \int_{-\infty}^{+\infty} \left| \frac{\partial v}{\partial \varphi} \right|_{\rho, z(t)} dt \leqslant \frac{1}{4} \beta \frac{\omega^*}{\omega} e^{-[\omega/\omega^*]} \tag{3.14}$$

On the other hand, by (3.12c) and (2.15a), at $t = \pm\infty$ one has $I = I'$, so that the inequality (3.13) is quite obvious, provided $p(t)$, $I(t)$ do not escape their domains. This condition, however, is immediately verified if one proceeds as in Corollary 1. ∎

4. THE POINT-MASS LIMIT

4.1. The Perturbative Treatment

We consider now the case of a small "molecule" of diameter proportional to a small parameter ε. Since the moment of inertia scales as ε^2, say one has $\mathscr{C}_\varepsilon = \varepsilon^2 C$, to keep finite the kinetic energy $I^2/2\varepsilon^2 C = \varepsilon^{-2} k(I)$ one needs $I \sim \varepsilon$, so that the angular velocity $\omega(I)$ grows as ε^{-1}.

We shall assume that the momentum $\partial v/\partial \varphi$ of the external forces is of order ε, as is the typical case for regular and purely positional forces; for instance, one could assume $v = v_0(q) + \varepsilon v_1(q, \varphi)$. We are thus led to study a Hamiltonian of the form

$$h(p, q, I, \varphi) = \varepsilon^{-2} k(I) + u(I, p, q, \varphi, \varepsilon) \tag{4.1}$$

with $\partial u/\partial \varphi = \mathcal{O}(\varepsilon)$, analytic in an ($\varepsilon$-dependent) real domain $\mathscr{D}_0 = \mathscr{B} \times \mathscr{I}_\varepsilon \times S^1$; here, $(p, q) \in \mathscr{B}$, a domain in $\mathbb{R}^{2n}$, $I \in \mathscr{I}_\varepsilon$, a real interval (or a point) which reduces to $\{0\}$ linearly with ε, and $\varphi \in S^1$.

We introduce, as in Section 2, the (now ε-dependent) complex sets $\Delta_{\rho,z}$, Δ_ρ, $\mathscr{S}_\rho$, and $\mathscr{D}_\rho$, with an (ε-dependent) vector $\rho = \rho(\varepsilon)$ given by

$$\rho = (\rho_p, \rho_q, \rho_I(\varepsilon), \rho_\varphi), \qquad \rho_I(\varepsilon) = \varepsilon \rho_I^0 \tag{4.2}$$

We assume $\rho_\varphi \leqslant 1$ and put

$$\rho_0^2 = \min(\rho_p \rho_q, \rho_\varphi \rho_I^0) \tag{4.3}$$

With reference to such domains, we use as above the supremum norm $|\cdot|_\sigma$, while for any function w the "vector field norm" is now defined in a slightly different way, by

$$\|w\|_\sigma = \max\left(\rho_q \left|\frac{\partial w}{\partial q}\right|_\sigma, \rho_p \left|\frac{\partial w}{\partial p}\right|_\sigma, \rho_I^0 \left|\frac{\partial w}{\partial I}\right|_\sigma, \rho_\varphi \left|\frac{\partial w}{\partial \varphi}\right|_\sigma\right) \tag{4.4}$$

We assume that h is analytic in $\mathscr{D}_\rho$. Moreover [since $\partial u/\partial\varphi = \mathcal{O}(\varepsilon)$ and $\rho_I = \varepsilon\rho_I^0$] we assume that there exists a quantity $\mathscr{U}_z$, $z \in \Delta_0$, such that one has

$$\rho_\varphi \left|\frac{\partial u}{\partial \varphi}\right|_\rho \leqslant \varepsilon\mathscr{U}_z, \qquad \rho_I^0 \left|\frac{\partial u}{\partial I}\right|_\rho \leqslant \mathscr{U}_z, \qquad \rho_a \left|\frac{\partial u}{\partial a}\right|_{\rho,z} \leqslant \mathscr{U}_z \qquad (a = p, q, I) \tag{4.5}$$

for every $z \in \Delta_0$. Notice that (4.5) implies $\|u\|_{\rho,z} \leqslant \mathscr{U}_z$. We shall denote $\mathscr{U} = \sup_{z \in \Delta_0} \mathscr{U}_z$. We introduce the constants Ω and C by

$$\varepsilon\Omega = \inf_{I \in \Delta_\rho} \left|\frac{\partial k}{\partial I}(I)\right|, \qquad C^{-1} = \left|\frac{\partial^2 k}{\partial I^2}\right|_\rho \tag{4.6}$$

and assume [having in mind the case of $k(I)$ quadratic in I] that both Ω and C remain finite and different from 0 for $\varepsilon \to 0$. Finally, for technical reasons, we also assume (as is not restrictive)

$$\rho_I^0 \leqslant \tfrac{1}{4} C\Omega\rho_\varphi \tag{4.7}$$

We can now state the following result.

Proposition 2. Within the above assumptions, let

$$\varepsilon \leqslant \varepsilon^* = 2^{-9}\rho_0^2\Omega\mathscr{U}^{-1} \tag{4.8}$$

Then there exists an analytic canonical transformation $\mathscr{C}: \mathscr{D}_{\frac{1}{2}\rho} \to \mathscr{D}_\rho$, $(z, \varphi) = \mathscr{C}(z', \varphi')$, which conjugates h to

$$h' = \varepsilon^{-2}k(I') + g(I', p', q') + e^{-[\varepsilon^*/\varepsilon]} f(p', q', I', \varphi') \tag{4.9}$$

with

$$\rho_\varphi \left|\frac{\partial f}{\partial \varphi}\right|_{\frac{1}{2}\rho, z} \leqslant \varepsilon\mathscr{U}_z \tag{4.10}$$

Moreover, one has

$$|I' - I| \leqslant 2^{-5} \frac{\varepsilon^2}{\varepsilon^*} \rho_I^0 \tag{4.11}$$

For the proof of this Proposition, see Section 5.3.

4.2. Applications

From Proposition 2 one can deduce two corollaries, corresponding to those of the previous section, for Hamiltonians of the form

$$h = \frac{I^2}{2C\varepsilon^2} + \frac{p^2}{2m} + v(q, \varphi) \tag{4.12}$$

with, for instance, $v = v_0(q) + \varepsilon v_1(q, \varphi)$; neglecting some details for brevity, let us only give a sketch of them.

(a) For the case of a bounded potential $v(q, \varphi)$, let E_0 be the initial value of the rotational energy, so that $I(0) = \varepsilon(2CE_0)^{1/2}$, and take $\mathscr{I}_\varepsilon = \{I(0)\}$; then, for not too large values of $p(0)^2/2m$, one finds

$$\begin{aligned} &|I(t) - I(0)| \leqslant \gamma_1 \frac{\varepsilon}{\varepsilon^*} |I(0)| = \gamma_2 \frac{\varepsilon^2}{\varepsilon^*} E_0 \\ &\left| \frac{I^2(t)}{2C\varepsilon^2} - E_0 \right| \leqslant \gamma_3 \frac{\varepsilon}{\varepsilon^*} E_0 \end{aligned} \tag{4.13}$$

for times $|t| = \gamma_4 \varepsilon \exp[\varepsilon^*/\varepsilon]$; $\gamma_1, \gamma_2,...$ are here positive constants, which could be easily computed. Notice that, because of the smallness of the body, the fluctuation $v - \bar{v}$ of the potential does not enter the balance of the rotational energy.

(b) For the case of scattering, working as in the previous case, one is led to

$$\left| \frac{I^2(+\infty)}{2C\varepsilon^2} - \frac{I^2(-\infty)}{2C\varepsilon^2} \right| \leqslant \gamma_5 e^{-[\varepsilon^*/\varepsilon]} \tag{4.14}$$

with suitable γ_5.

5. PROOF OF PROPOSITIONS 1 AND 2

5.1. The Iterative Lemma

In order to prove Proposition 1, we regard the Hamiltonian $h = k + u$ as a perturbation of $k + \bar{u}$, and construct a sequence of "normalizing" canonical transformations, each gaining an order in Ω^*/Ω. Since we need an explicit estimate for the term of order Ω^*/Ω in h', we treat the first perturbative step separately.

We work directly on the Hamiltonian vector fields, and not only on Hamilton functions. As shown in ref. 19, this procedure gives some advantage. Indeed, with small additional price, it leads to pure exponentials of the form $\exp(-\Omega/\Omega^*)$ instead of $\exp[-(\Omega/\Omega^*)^{1/2}]$, as in ref. 9 (see, however, ref. 10).

As a rule, we denote functions by lowercase letters, and their Hamiltonian vector fields by the corresponding capital letters. For a Hamiltonian vector field W, corresponding to the Hamilton function w, we denote $\|W\|_\sigma = \|w\|_\sigma$, i.e.,

$$\|W\|_\sigma = \max_{a=p,q,I,\varphi} \rho_{\bar{a}} \, |W^a|_\sigma \tag{5.1}$$

$\bar{a}$ denoting the conjugate variable of a. A similar notation is used for the local norm $\|W\|_{\sigma,z}$.

The proof of Proposition 1 is a consequence of the following lemma, which, up to details, is quite typical in perturbation theory.

Lemma 1 (On the normal form). Let the function

$$h(p,q,I,\varphi) = k(I) + g(p,q,I) + f(p,q,I,\varphi) \tag{5.2}$$

be analytic and bounded, together with its Hamiltonian vector field $H = K + G + F$, in the domain $\mathscr{D}_\sigma$ $(\sigma \leqslant \rho)$. Fix any positive number α such that $\alpha\rho < \sigma$, and assume

$$\Omega \geqslant \max\left(\frac{2^6\,\|F\|_\sigma}{\alpha\rho^2}, \frac{8\rho_I}{C\rho_\varphi}\right) \tag{5.3}$$

C being defined as in (2.10). Then, there exists a real analytic canonical transformation $\Phi: \mathscr{D}_{\sigma-\alpha\rho} \to \mathscr{D}_\sigma$ which conjugates h to $h' = k + g' + f'$, with $g' = g + \bar{f}$; the function f' and its Hamiltonian vector field F' satisfy, for any $z \in \Delta_0$ and $a = p, q, I$, the local estimates

$$\begin{aligned} |F'^a|_{\sigma-\alpha\rho,z} \leqslant \frac{16}{\alpha\Omega\rho^2} &[\|F\|_{\sigma,z}(|G^a|_{\sigma,z} + 2\,|F^a|_{\sigma,z}) \\ &+ |F^a|_{\sigma,z}(\|G\|_{\sigma,z} + 2\,\|F\|_{\sigma,z})] \end{aligned} \tag{5.4a}$$

$$\rho_I\,|F'^\varphi|_{\sigma-\alpha\rho,z} \leqslant \frac{32}{\alpha\Omega\rho^2}\,\|F\|_{\sigma,z}(\|G\|_{\sigma,z} + 2\,\|F\|_{\sigma,z}) \tag{5.4b}$$

$$|f'|_{\sigma-\alpha\rho,z} \leqslant \frac{8}{\alpha\Omega\rho^2}\,(\|G\|_{\sigma,z} + 2\,\|F\|_{\sigma,z})\,|f - \bar{f}|_{\sigma,z} \tag{5.4c}$$

Furthermore, denoting $(z, \varphi) = \Phi(z', \varphi')$, one has

$$\begin{aligned} |a' - a| &\leqslant \frac{8}{\Omega} |F^a|_{\sigma,z} \qquad (a = p, q, I) \\ \rho_I |\varphi' - \varphi| &\leqslant \frac{8}{\Omega} \|F\|_{\sigma,z} \end{aligned} \tag{5.5}$$

and also, for any function $w: \mathscr{D}_\sigma \to \mathbb{C}$,

$$|w \circ \Phi - w|_{\sigma - \alpha\rho, z} \leqslant \frac{16}{\alpha\Omega\rho^2} \|F\|_{\sigma,z} |w|_{\sigma,z} \tag{5.6}$$

Proof. We construct Φ as the time-one map Φ_1^X of a suitable Hamiltonian vector field X. This is the Lie method, which is briefly recounted in the Appendix; the relevant estimates are there reported in two technical lemmas. Let us here recall that for any function w and any vector field W, one has

$$\begin{aligned} (\Phi_1^X)^* w &= w + \mathscr{R}_1^X(w) = w + L_X w + \mathscr{R}_2^X(w) \\ (\Phi_1^X)^* W &= W + \mathscr{R}_1^X(W) = W + L_X W + \mathscr{R}_2^X(W) \end{aligned} \tag{5.7}$$

where L_X is the Lie derivative associated with the vector field X, while $\Phi^* w = w \circ \Phi$ and $\Phi^* W = ((D\Phi^{-1}) W) \circ \Phi$ are the pullbacks of w and W, respectively, and $\mathscr{R}_k^X$, $k = 1, 2$, denotes the kth remainder of the Lie series, defined as in (A.4) [roughly speaking, $\mathscr{R}_k^X(W)$ is as small as $\|X\|^k \, \|W\|$].

In order to normalize H, the vector field X is chosen so to satisfy the equation

$$L_K X = F - \bar{F} \tag{5.8}$$

Indeed, after this choice one gets for $H' = (\Phi_1^X)^* H$ the form $K + G' + F'$, with $G' = G + \bar{F}$ and

$$F' = \mathscr{R}_1^X(G + F) + \mathscr{R}_2^X(K) \tag{5.9}$$

and it is not difficult to recognize that both X and F' turn out to be proportional to Ω^{-1}. More precisely, since $K = K^\varphi(I)\, \partial_\varphi$, Eq. (5.8) reads in components

$$\begin{aligned} K^\varphi \frac{\partial X^a}{\partial \varphi} &= F^a - \bar{F}^a \qquad (a = p, q, I) \\ K^\varphi \frac{\partial X^\varphi}{\partial \varphi} &= F^\varphi - \bar{F}^\varphi + X^I \frac{\partial K^\varphi}{\partial I} \end{aligned}$$

and is readily solved by

$$X^a = \frac{1}{K^\varphi} \int_0^\varphi (F^a - \bar{F}^a)\, d\varphi' \qquad (a = p, q, I)$$

$$X^\varphi = \frac{1}{K^\varphi} \int_0^\varphi (F^\varphi - \bar{F}^\varphi)\, d\varphi' + \left(\frac{1}{K^\varphi}\right)^2 \frac{\partial K^\varphi}{\partial I} \int_0^\varphi d\varphi' \int_0^{\varphi'} F^I\, d\varphi''$$

(use is made of $\bar{F}^I = 0$). Since $\Omega \leqslant |K^\varphi(I)|$ and $C^{-1} \geqslant |\partial_I K^\varphi(I)|$, one gets the estimates

$$|X^a|_{\sigma,z} \leqslant \frac{1}{\Omega} (\pi^2 + \rho_\varphi^2)^{1/2}\, |F^a - \bar{F}^a|_{\sigma,z} < \frac{4}{\Omega} |F^a - \bar{F}^a|_{\sigma,z} \qquad (a = p, q, I)$$

$$\begin{aligned} |X^\varphi|_{\sigma,z} &\leqslant \frac{1}{\Omega} (\pi^2 + \rho_\varphi^2)^{1/2}\, |F^\varphi - \bar{F}^\varphi|_{\sigma,z} + \frac{1}{2C\Omega^2} (\pi^2 + \rho_\varphi^2)\, |F^I - \bar{F}^I|_{\sigma,z} \qquad (5.10) \\ &< \frac{4}{\Omega \rho_I} \|F - \bar{F}\|_{\sigma,z} \end{aligned}$$

(use is made of $\rho_\varphi \leqslant 1$ and $\Omega \geqslant 8\rho_I / C\rho_\varphi$), and then also

$$\|X\|_{\sigma,z} \leqslant 4\Omega^{-1} \|F - \bar{F}\|_{\sigma,z} \leqslant 8\Omega^{-1} \|F\|_{\sigma,z} \qquad (5.11)$$

We now make use of Lemma A2 of the Appendix. First of all, from this lemma one knows that Φ_1^X is well defined, and properly estimated, provided $\|X\|_\sigma \leqslant \alpha\rho^2/8$; by (5.11) and (5.3) this condition is fulfilled. Furthermore, the estimates (5.5) follow from (5.10), since one has $|\Phi_1^X(z)_a - a| \leqslant |X^a|_{\sigma,z}$, while (5.6) is a consequence of (A.6b) and (A.5a).

Let us now prove the estimates (5.4). First, from (5.10) and from the estimate (A.6a) of Lemma A2, one gets, for $a = p, q, I$,

$$\begin{aligned} &|[\mathscr{R}_1^X(G + F)]^a|_{\sigma - \alpha\rho, z} \\ &\quad \leqslant \frac{8}{\alpha\Omega\rho^2} [\, \|F - \bar{F}\|_{\sigma,z}\, |G^a + F^a|_{\sigma,z} + |F^a - \bar{F}^a|_{\sigma,z}\, \|G + F\|_{\sigma,z}] \end{aligned}$$

On the other hand, using (5.8), the estimates (A.5a) and (5.3) give

$$\begin{aligned} |[\mathscr{R}_2^X(K)]^a|_{\sigma - \alpha\rho, z} &\leqslant \sum_{j=2}^\infty \frac{1}{j!} |[L_X^{j-1}(F - \bar{F})]^a|_{\sigma - \alpha\rho, z} \\ &\leqslant \frac{8}{\alpha\Omega\rho^2} \|F - \bar{F}\|_{\sigma,z}\, |F^a - \bar{F}^a|_{\sigma,z} \end{aligned}$$

This proves (5.4a); (5.4b) is proven similarly.

Finally, let us notice that the vector field X is Hamiltonian, with Hamilton function

$$\chi = \frac{1}{K^\varphi} \int_0^\varphi (f - \bar{f})\, d\varphi'$$

Thus, Φ_1^X is canonical, and the new Hamiltonian $h' = h \circ \Phi_1^X$ has indeed the form $k + g' + f'$, with $g' = g + \bar{f}$ and $f' = \mathscr{R}_1^X(g + f) + \mathscr{R}_2^X(k)$. Moreover, the function χ satisfies $|\chi|_{\sigma,z} \leqslant 4\Omega^{-1} |f - \bar{f}|_{\sigma,z}$. Thus, (5.4c) follows from (A.6b) (A.6c), using also $L_X(g + f) = -L_{(G+F)}\chi$, $L_X w = f - \bar{f}$, and (A.5a). ∎

5.2. Proof of Proposition 1

Let us denote by $H_{-1} = K + G_{-1} + F_{-1}$ the Hamiltonian vector field of the Hamilton function h given by (2.1), with $G_{-1} = 0$ and $F_{-1} = U$, U being the Hamiltonian vector field of the function u. We apply a first time Lemma 1 to H_{-1}, with $\alpha = 1/4$ and $\sigma = \rho$. This is possible, since in this case (5.3) is implied by (2.11). In such a way, we construct a first canonical transformation $\mathscr{C}_{-1}$, which gives the new vector field $H_0 = \mathscr{C}_{-1}^* H_{-1}$ the form

$$H_0 = K + G_0 + F_0$$

with $G_0 = \bar{U}$, while F_0 and its Hamilton function f_0 satisfy the estimates

$$|F_0^a|_{\frac{3}{4}\rho,z} \leqslant \frac{1}{4} \frac{\Omega^*}{\Omega} |U^a|_{\rho,z} \qquad (a = p, q, I) \tag{5.12a}$$

$$\rho_I\, |F_0^\varphi|_{\frac{3}{4}\rho,z} \leqslant \frac{1}{4} \frac{\Omega^*}{\Omega} \|U\|_{\rho,z} \tag{5.12b}$$

$$|f_0|_{\frac{3}{4}\rho,z} \leqslant \frac{1}{16} \frac{\Omega^*}{\Omega} |u - \bar{u}|_{\rho,z} \tag{5.12c}$$

We can now apply r times Lemma 1, each time with $\alpha = 1/(4r)$, thus constructing the Hamilton functions $h_{s+1} = h_s \circ \mathscr{C}_s$ and the corresponding vector fields H_{s+1}, $s = 0, 1, \ldots, r-1$. Actually, it is enough to use here the inequalities of Lemma 1, with $\|F - \bar{F}\|$ and $|F^a - \bar{F}^a|$ replaced everywhere by $2\,\|F\|$ and, respectively, $2\,|F^a|$. Let us write $\rho_s = (3/4 - s/4r)\rho$; proceeding inductively, one shows that after s steps, one gets a Hamiltonian vector field H_s of the form $H_s = K + G_s + F_s$, $s = 1, \ldots, r$, with

$$G_s = G_0 + \sum_{j=0}^{s-1} \bar{F}_j \tag{5.13a}$$

$$|F_s^a|_{\rho_s, z} \leqslant \frac{1}{4} \frac{\Omega^*}{\Omega} |U^a|_{\rho, z} e^{-s} \qquad (a = p, q, I) \tag{5.13b}$$

$$\rho_I |F_s^\varphi|_{\rho_s, z} \leqslant \frac{1}{4} \frac{\Omega^*}{\Omega} \|U\|_{\rho, z} e^{-s} \tag{5.13c}$$

Indeed, by (5.12), these relations are true for $s = 0$. Assume then that s steps have been performed. If $\Omega \geqslant (2^8 r/\rho^2) \|F_s\|_{\rho_s}$, we can apply once more Lemma 1, arriving at $H_{s+1} = K + G_{s+1} + F_{s+1}$, with G_{s+1} still of the form (5.13a) and F_{s+1} satisfying

$$|F_{s+1}^a|_{\rho_{s+1}, z} \leqslant \frac{2^6 r}{\Omega \rho^2} [\|F_s\|_{\rho_s, z}(|G_s^a|_{\rho_s, z} + 2 |F_s^a|_{\rho_s, z})$$

$$+ |F_s^a|_{\rho_s, z}(\|G_s\|_{\rho_s, z} + 2 \|F_s\|_{\rho_s, z})] \tag{5.14}$$

with a similar estimate for the φ component. Let us now observe that, by (5.13b), one has

$$|G_s^a|_{\rho_s, z} + 2 |F_s^a|_{\rho_s, z} \leqslant |G_0^a|_{\rho, z} + |F_s^a|_{\rho_s, z} + \sum_{j=0}^{s} |F_j^a|_{\rho_j, z} < \frac{3}{2} |U^a|_{\rho, z} \tag{5.15}$$

Then, from (5.14) we see that the inequalities (5.13b) and (5.13c) are true also for $s + 1$, provided $(3/16)(\Omega^*/\Omega) r \leqslant 1/\varepsilon$. In order to satisfy this condition, we simply choose $r = [\Omega/\Omega^*]$. Notice that with such a value of r, one has also $\Omega \geqslant (2^8 r/\rho^2) \|F_j\|_{\rho_j}$ for all $j = 0, 1, \ldots, s + 1$.

In such a way, one constructs the final Hamiltonian $h_r = k + g_r + f_r$. This coincides with h' given by (2.13), g_r and f_r being related to g and f via $g_r = \bar{u} + (\Omega^*/\Omega) g$, $f_r = (\Omega^*/\Omega) e^{-[\Omega/\Omega^*]} f$. Then (2.14c) follows from (5.13b). Concerning the estimates (2.14a), (2.14b), it is sufficient to notice that (5.4c), (5.13), and (5.15) imply

$$|f_{s+1}|_{\rho_{s+1}, z} \leqslant 2^7 \frac{\|U\|_\rho}{\Omega \rho^2} r |f_s|_{\rho_s, z} \leqslant \frac{1}{8} |f_s|_{\rho_s, z}$$

to conclude

$$|f_s|_{\rho_s, z} \leqslant 2^{-3s} \frac{\Omega^*}{10\Omega} |u - \bar{u}|_{\rho, z}$$

This proves (2.14b), since $r \geqslant 1$. From $|g_r - \bar{u}|_{\frac{1}{2}\rho, z} \leqslant \sum_{j=0}^{r-1} |f_j|_{\rho_j, z}$ one then deduces (2.14a).

Finally, the estimates (2.15) on the overall canonical transformation $\mathscr{C} = \mathscr{C}_{-1} \circ \mathscr{C}_0 \circ \cdots \circ \mathscr{C}_{r-1}$ are easy consequences of (5.5), (5.6), (5.12), and (5.13). ∎

5.3. Proof of Proposition 2

The proof of Proposition 2 differs only slightly from the proof of Proposition 1. We work in domains $\mathscr{D}_\sigma \subset \mathscr{D}_\rho$, the extension σ now depending (as ρ) on ε through its I component, namely

$$\sigma(\varepsilon) = (\sigma_p, \sigma_q, \sigma_I(\varepsilon), \sigma_\varphi) \leqslant \rho(\varepsilon), \qquad \sigma_I(\varepsilon) = \varepsilon\sigma_I^0$$

In these domains we use for vector fields the norm

$$\|W\|_\sigma = \max_{a = p, q, I, \varphi} \rho_{\bar{a}}^0 \, |W^a|_\sigma$$

where $\rho_a^0 = \rho_a$ for $a \neq I$. We then consider the Hamiltonian vector field $H = \varepsilon^{-2}K + G + F$, analytic in $\mathscr{D}_\sigma$, which is assumed to satisfy $G^I = 0$, $\rho_\varphi \, |F^I|_{\sigma,z} \leqslant \varepsilon \mathscr{F}_z$, and $\|F\|_{\sigma,z} \leqslant \mathscr{F}_z$.

The following lemma replaces Lemma 1:

Lemma 2. In addition to (4.6) and (4.7), assume

$$\varepsilon \leqslant 2^{-6}\alpha\Omega\rho_0^2\mathscr{F}^{-1}$$

Then there exists an analytic canonical transformation Φ: $\mathscr{D}_{\sigma-\alpha\rho} \to \mathscr{D}_\sigma$ such that one has $\Phi^*H = \varepsilon^{-2}K + G' + F'$, with $G' = G + \bar{F}$ and

$$|F'^a|_{\sigma-\alpha\rho,z} \leqslant \frac{2^4\varepsilon}{\alpha\Omega\rho_0^2}\,[\,|F^a|_{\sigma,z}(\|G\|_{\sigma,z} + 2\mathscr{F}_z)$$
$$+ \mathscr{F}_z(|G^a|_{\sigma,z} + 2\,|F^a|_{\sigma,z})] \qquad (a = p, q, I)$$

$$|F'^\varphi|_{\sigma-\alpha\rho,z} \leqslant \frac{2^5\varepsilon}{\alpha\Omega\rho_0^2}\,\mathscr{F}_z(\|G\|_{\sigma,z} + 2\mathscr{F}_z)$$

Furthermore, writing $(z, \varphi) = \Phi(z', \varphi')$, one has, for $z \in \Delta_0$,

$$|a' - a| \leqslant \frac{8\varepsilon}{\Omega}\,|F^a|_\sigma \qquad (a = p, q, I)$$

The proof of Lemma 2 goes the same way as for Lemma 1, with the following differences. Let $\Phi = \Phi_1^X$, with X defined by the equation $L_K X = \varepsilon^2(F - \bar{F})$; one has now the estimates

$$|X^a|_{\sigma,z} \leqslant \frac{8\varepsilon}{\Omega}\,|F^a|_{\sigma,z} \leqslant \frac{8\varepsilon\mathscr{F}_z}{\Omega\rho_{\bar{a}}} \qquad (a = p, q)$$

$$|X^I|_{\sigma,z} \leqslant \frac{8\varepsilon^2\mathscr{F}_z}{\Omega\rho_\varphi}$$

$$|X^\varphi|_{\sigma,z} \leqslant \frac{8\varepsilon\mathscr{F}_z}{\Omega\rho_I^0}$$

The key point is that one has

$$\max_b \frac{|F^b|_{\sigma,z}}{\alpha\rho_b} \leqslant \frac{\mathscr{F}_z}{\alpha\rho_0^2}, \qquad \max_b \frac{|G^b|_{\sigma,z}}{\alpha\rho_b} \leqslant \frac{\|G\|_{\sigma,z}}{\alpha\rho_0^2}$$

and also

$$\max_b \frac{|X^b|_{\sigma,z}}{\alpha\rho_b} \leqslant \frac{8\varepsilon\mathscr{F}_z}{\alpha\Omega\rho_0^2}$$

Proposition 2 is then obtained by iterating the construction of Lemma 2, with $\alpha = 1/(2r)$ and $r = [\varepsilon^*/\varepsilon]$.

6. CONCLUSIONS: SOME CRITICISM, AND OPEN PROBLEMS

The Boltzmann–Jeans conjecture on the classical "freezing" of fast rotations was here proven, although in connection with a rather particular class of models. Unfortunately, for several important reasons our results are yet too poor for a physical interpretation. First of all, the planar problem we deal with is physically dissatisfying. The corresponding three-dimensional problem, that is, the problem of the energy exchanges between the translational and the rotational degrees of freedom of a fast rotating rigid body, is obviously more difficult, but certainly much more interesting. Work is in progress in this direction; in fact, we are convinced that the exponential laws (1.2) and (1.3), if conveniently adapted (and somehow worsened), also hold for the three-dimensioal problem, at least in the case of the point-mass limit.

Let us also remark that even in the planar case we are still far from a complete understanding of the Boltzmann–Jeans conjecture. For example, it would be important to study a model including simultaneously fast rotations and fast vibrations. This means that one should develop a perturbative scheme with two parameters, and go beyond the usual decomposition of the variables into fast and slow ones, by introducing (for rotations) an intermediate class. As a result, one should be able to put in evidence different freezing phenomena, occurring at different time scales. Still, in view of the physical understanding, one should also study, in addition to the molecule–wall collision, the collisions between two or more rotating molecules (the corresponding problem for purely vibrating molecules was studied in ref. 10). As a matter of fact, such a problem turns out to be technically related to the study of the three-dimensional rotations, so we hope to be able to treat both problems at the same time.

As a final remark, let us make a comment on the relation between the present paper and ref. 16, where, as recalled in the Introduction, one studies numerically a particular Hamiltonian system belonging to the class considered here, namely of the form (1.1). One could simply say that we did prove here some of the results exhibited there (apart from the estimate of the constants,[5] which, as is typical of classical perturbation theory, is somehow dissatisfying). But in fact, it is quite evident that, even qualitatively, our analytic results are somehow poor if compared with the richer phenomenology revealed by the numerical simulation. Although some relevant phenomena (in particular, the presence of two different exponential laws for the maximum energy exchange and for its average on the initial phase) can be certainly explained by a more careful use of the transformed Hamiltonian, in our opinion it is not definitely clear whether perturbation theory alone can lead to a full understanding of the problem, and in general of the Boltzmann–Jeans conjecture. Our feeling is that some other tools, for example, some rigorous version of the already quoted heuristic approach by Jeans, Landau–Teller, and Rapp, should also be taken into consideration. We hope to come back to this question in a forthcoming paper.

APPENDIX: THE LIE METHOD

We give here a sketch of the Lie method for vector fields; for more details and general references, see ref. 19. The Lie method is a transformation theory based on the realization of (canonical) diffeomorphisms close to the identity, as flows of (Hamiltonian) vector fields. Let us denote by Φ_τ^X the map at time τ associated to the vector field X. At the basis of the method there are the well-known identities

$$\frac{d}{d\tau}(\Phi_\tau^X)^* \, w = (\Phi_\tau^X)^* \, L_X w \tag{A.1a}$$

$$\frac{d}{d\tau}(\Phi_\tau^X)^* \, W = (\Phi_\tau^X)^* \, L_X W \tag{A.1b}$$

relating time derivatives along the flow to Lie derivatives. Here, $\Phi^* w = w \circ \Phi$ and $\Phi^* W = ((D\Phi^{-1}) W) \circ \Phi$ denote, respectively, the pullbacks of the function w and of the vector field W under the mapping Φ. Let us also

[5] It would not be difficult, although somehow annoying, to improve the numerical constants appearing in (2.12) and (4.8) by, say, a factor 10. Of course, this does not change the essence of the problem.

recall that the Lie derivative L_X acts on functions and on vector fields, respectively, according to

$$L_X w = \sum_a X^a \frac{\partial w}{\partial a} \tag{A.2a}$$

$$(L_X W)^a = L_X W^a - L_W X^a \tag{A.2b}$$

An iterated use of (A.2b) leads in a trivial way to the "Lie series" representation of the "Lie transform" $W \mapsto (\Phi_1^X)^* W$:

$$(\Phi_1^X)^* W = \sum_{s=0}^{\infty} \frac{1}{s!} L_X^s W \tag{A.3}$$

In the analytic case, the convergence of such a series expansion is easily established (see Lemma A1 below). For any $k = 1, 2,...$, the kth remainder $\mathscr{R}_k^X(W)$ of the Lie series (A.3) is defined by

$$R_k^X W = \sum_{s=k}^{\infty} \frac{1}{s!} L_X^s W \tag{A.4}$$

Completely analogous expansions are obtained for functions.

We now produce two lemmas, reporting some rigorous estimates on the Lie series; detailed proofs can be found in ref. 19. We consider a function w and two vector fields X and W, defined and analytic in the domain $\mathscr{D}_\rho$; σ, ρ, and α are as above. We refer to the supremum local norm (2.6).

Lemma A1 (On Lie derivatives). For any $z \in \Delta_0$ and any $s = 1, 2,...$, one has

$$|L_X w|_{\sigma - \alpha\rho, z} \leqslant \left(\max_b \frac{|X^b|_{\sigma - \alpha\rho, z}}{\alpha\rho_b} \right) |w|_{\sigma, z} \tag{A.5a}$$

$$\frac{1}{s!} |(L_X^s W)^a|_{\sigma - \alpha\rho} \leqslant \left(4 \max_b \frac{|X^b|_{\sigma, z}}{\alpha\rho_b} \right)^{s-1} \times \left[|X^a|_{\sigma, z} \max_b \frac{|W^b|_{\sigma, z}}{\alpha\rho_b} + |W^a|_{\sigma, z} \max_b \frac{|X^b|_{\sigma, z}}{\alpha\rho_b} \right] \tag{A.5b}$$

Sketch of the Proof. The inequality (A.5a) is simply proven by a Cauchy estimate of the time derivative at the lhs of (A.1a). Concerning (A.5b), one uses instead (A.2b), (A.5a), and an inductive procedure. ∎

Lemma A2 (On Lie transforms). Assume $|X^a|_\sigma \leqslant \alpha\rho^a/8$, for $a = p, q, I, \varphi$. Then:

(i) The mapping $\Phi_1^X\colon \mathscr{D}_{\sigma-\alpha\rho} \to \Phi_1^X(\mathscr{D}_{\sigma-\alpha\rho}) \subset \mathscr{D}_\sigma$ is an analytic diffeomorphism, and for each $z \in \Delta_0$ one has $\Phi_1^X(\mathscr{D}_{\sigma-\alpha\rho,z}) \subset \mathscr{D}_{\sigma-\frac{1}{2}\alpha\rho,z}$.

(ii) The vector field $(\Phi_1^X)^* W$ and the function $(\Phi_1^X)^* w$ are analytic in $\mathscr{D}_{\sigma-\alpha\rho}$, and one has, for any $z \in \Delta_0$:

$$|(\mathscr{R}_1^X W)^a|_{\sigma-\alpha\rho,z} \leqslant 2\left[|X^a|_{\sigma,z} \max_b \frac{|W^b|_{\sigma,z}}{\alpha\rho_b} + |W^a|_{\sigma,z} \max_b \frac{|X^b|_{\sigma,z}}{\alpha\rho_b}\right] \tag{A.6a}$$

$$|\mathscr{R}_1^X w|_{\sigma-\alpha\rho,z} \leqslant |L_X w|_{\sigma-\frac{1}{2}\alpha\rho,z} \tag{A.6b}$$

$$|\mathscr{R}_2^X w|_{\sigma-\alpha\rho,z} \leqslant \frac{1}{2}\,|L_X^2 w|_{\sigma-\frac{1}{2}\alpha\rho,z} \tag{A.6c}$$

Sketch of the Proof. The statement (i) is an elementary consequence of general properties of ordinary differential equations; in particular, the inclusion property for $\Phi_1^X(\mathscr{D}_{\sigma-\alpha\rho,z})$ follows from the *a priori* estimate $|(\Phi_1^X z)_a - a| \leqslant |X^a|$. The estimate (A.6a) is obtained in a simple way using (A.3) and (A.5b). Finally, (A.6b), (A.6c) follow from writing $\mathscr{R}_1^X(w) = \int_0^1 (L_X w)\circ\Phi_\tau^X\,d\tau$ and $\mathscr{R}_2^X(w) = \int_0^1 d\tau' \int_0^\tau (L_X^2 w)\circ\Phi_{\tau'}^X\,d\tau'$. ∎

Remark. Using the norm (5.1), the inequalities appearing in Lemmas A1 and A2 take the slightly more compact form

$$|L_X w|_{\sigma-\alpha\rho,z} \leqslant \frac{\|X\|_{\sigma-\alpha\rho,z}}{\alpha\rho^2}\,|w|_{\sigma,z} \tag{A.7a}$$

$$\begin{aligned}\frac{1}{s!}\,|(L_X^s W)^a|_{\sigma-\alpha\rho,z} \leqslant{}& \frac{1}{\alpha\rho^2}\left(\frac{4\,\|X\|_{\sigma,z}}{\alpha\rho^2}\right)^{s-1} \\ &\times [\,|X^a|_{\sigma,z}\,\|W\|_{\sigma,z} + |W^a|_{\sigma,z}\,\|X\|_{\sigma,z}]\end{aligned} \tag{A.7b}$$

$$|(\mathscr{R}_1^X W)^a|_{\sigma-\alpha\rho,z} \leqslant \frac{2}{\alpha\rho^2}\,[\,|X^a|_{\sigma,z}\,\|W\|_{\sigma,z} + |W^a|_{\sigma,z}\,\|X\|_{\sigma,z}] \tag{A.7c}$$

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