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On the Landau–Teller Approximation for Energy Exchanges with Fast Degrees of Freedom

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We revisit the Landau–Teller heuristic approach to adiabatic invariants and, following Rapp, use it to investigate the energy exchanges between the different degrees of freedom, in simple Hamiltonian systems describing the collision of fast rotating or vibrating molecules with a fixed wall. We critically compare the theoretical results with particularly accurate numerical computations (quite small energy exchanges, namely of one part over 10^{30}, are measured).

KEY WORDS: Energy sharing; molecular collisions; equilibrium times; adiabatic invariants; Landau–Teller method; numerical simulation.

1. INTRODUCTION

The problem of estimating the energy exchanges between fast and slow degrees of freedom is a very relevant one in many domains of physics, and is in fact the main motivation for the study of adiabatic invariants. Different approaches lead, in the analytic case and for a single fast degree of freedom of frequency ω, to exponential estimates of the form

$$|\Delta E| < \mathscr{E} e^{-\lambda\omega}, \qquad \mathscr{E}, \lambda > 0 \tag{1.1}$$

A rigorous mathematical scheme, leading in particular to the above law, is provided by classical perturbation theory[1,2] (see ref. 3 for a particular extension to the case of several oscillators). As is well known, perturbative

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methods are quite general and powerful, and at least in some cases they likely lead to optimal qualitative results: unfortunately, however, the estimates one gets for the constants—in particular, in the problem at hand, for λ, which is the most relevant one—are terribly pessimistic, and certainly far from optimal.

An interesting heuristic approach to the problem, also leading to the above exponential law, was proposed in 1936 by Landau and Teller[4] (in fact, the essential ideas go back to Jeans[5,6]). To illustrate the method, let us consider a particular application due to Rapp,[7,8] where one considers the problem of the collinear collision of a diatomic molecule with a point mass, or equivalently with a fixed obstacle (for an application to plasma physics, see refs. 9 and 10). After some preliminary work, Rapp is led to consider the particular Hamiltonian

$$H(x, y, p_x, p_y) = \tfrac{1}{2}p_x^2 + \tfrac{1}{2}(p_y^2 + \omega^2 y^2) + (1+y)\,e^{-x} \tag{1.2}$$

where x is the distance between the (center of mass of) the molecule and the colliding particle (or the obstacle), while y is the internal degree of freedom of the molecule, and p_x, p_y are the corresponding momenta. The equations of motion of the system are

$$\ddot{x} - e^{-x} = ye^{-x}, \qquad \ddot{y} + \omega^2 y = -e^{-x} \tag{1.3}$$

and one is interested in the energy ΔE acquired by the oscillator after the collision. Working on the equation for y by the so-called method of variation of arbitrary constants, one easily gets for ΔE the integral expression

$$\Delta E = (2E_0)^{1/2}\,|J|\cos\varphi_0 + \tfrac{1}{2}|J|^2, \qquad J = \int_{-\infty}^{\infty} e^{-x(t)}e^{-i\omega t}\,dt \tag{1.4}$$

where E_0 is the energy of the oscillator at $t = -\infty$, while $x(t)$ is the (unknown) motion of the x variable, and φ_0 is a convenient asymptotic phase (see ref. 7 or ref. 11 for details).

Now, the essence of the Landau–Teller method consists in replacing the true motion $x(t)$ inside the integral J by the free motion $\hat{x}(t)$, namely the solution of the equation

$$\ddot{x} - e^{-x} = 0$$

in which the internal degree of freedom y does not appear. At variance with the true solution $x(t)$, the approximated solution $\hat{x}(t)$ is independent of ω, so that J reduces to the Fourier transform of $e^{-\hat{x}(t)}$; as a consequence, in this analytic case, J decays exponentially with ω, and the coefficient of ω at the exponent turns out to coincide with the width τ of the analyticity

strip of $e^{-\hat{x}(t)}$ (thought of as function of the complex time t). In this approximation one then gets for ΔE an expression of the form

$$\Delta E = Ce^{-\tau\omega}\cos\varphi_0 + C'e^{-2\tau\omega} \tag{1.5}$$

which gives in particular the exponential law (1.1). For the particularly simple potential introduced in the model, τ is easily computed explicitly, and one gets $\tau = \pi/v_0$, where v_0 is the asymptotic value, at $t = -\infty$, of the velocity $d\hat{x}/dt$.

The Landau–Teller approximation has been successfully used in several occasions (see, for example, refs. 8 and 10); on the other hand, as explained in more detail in ref. 11, it is not so easy to provide for it a clear justification, and in particular to understand its range of applicability. In fact, only in a very particular case, namely when the initial energy E_0 practically vanishes, has the approximation been rigorously justified;[11] indeed, under this strong (but apparently unavoidable) assumption, one is able to prove that the width τ^* of the analyticity strip of the true solution $x(t)$, which in general depends on ω, tends[4] for large ω to the approximate value $\tau = \pi/v_0$. For $E_0 > 0$, as far as we know, no clear result is available.

The main purpose of the present paper is to make a *very accurate* numerical investigation of the reliability of the Landau–Teller approximation in the case $E_0 > 0$. More precisely, we first introduce a minor rearrangement in the approximation, which makes it suitable to treat a wider class of models, in particular a model including a fast rotator in place of an oscillator. From this modified scheme, we deduce the exponential law for the energy exchanges, with some further details not appearing in the original version of the approximation, and then compare these results with numerical computations; according to ref. 12, the use of a symplectic integration algorithm allows one to appreciate very small energy exchanges (*up to quantities, say, of one part over* 10^{30}), so the test is indeed quite accurate. As a result, one finds a really excellent agreement, at least with regard to the value of the coefficient λ, which is always found to coincide, for large ω, with the free value τ.

On the other hand, we also give a numerical estimate of the true analyticity width τ^*; as a matter of fact, we find that not only does τ^* not converge to τ for large ω, but it apparently tends to zero. This indicates in particular that the mechanism proposed in ref. 11 to justify the Landau–Teller approximation is not a general one. In fact, the situation is, in our opinion, a bit paradoxical, and the only conclusion we are able to draw is that the problem of understanding the Landau–Teller approximation should be still considered as essentially open.

[4] More precisely, a lower bound to τ^* tends to τ.

2. THE LANDAU-TELLER APPROXIMATION IN ACTION–ANGLE VARIABLES

Let us consider a Hamiltonian system of the form

$$H(I, \varphi, p, x) = h(I) + \frac{|p|^2}{2m} + f(I, \varphi, x) \tag{2.1}$$

with $I \in \mathbb{R}$, $\varphi \in S^1$, $(p, x) \in \mathbb{R}^{2n}$; we assume the interaction vanishes at infinity, more precisely

$$\lim_{|x| \to \infty} \frac{\partial f}{\partial x_i} = 0, \qquad i = 1, \ldots, n \tag{2.2}$$

Hamiltonian (1.2), after the introduction of the usual action–angle coordinates for the oscillator, is a particular case of Hamiltonian (2.1), for $n = 1$, $h(I) = \omega I$, and $f = e^{-x}[1 + (2I/\omega)^{1/2} \cos \varphi]$. Instead, for $h(I) = \frac{1}{2}I^2$ and some f independent of I, one describes the scattering of a rotator by a fixed obstacle.

The Landau–Teller approximation in these variables can be formulated as follows: consider an asymptotic state before the collision, say $p = p_0$, $x(t) = x_0 + p_0 t$, $I = I_0$, and

$$\varphi(t) = \omega t + \varphi_0, \qquad \omega = \frac{\partial h}{\partial I}(I_0) \tag{2.3}$$

Then proceed as follows:

(i) Replace the interaction potential f by its average $\bar{f}$ on φ, and introduce the free motion $\hat{p}(t)$, $\hat{x}(t)$ of the p, x variables, defined as the solution of the Hamiltonian problem

$$\hat{H}(p, x) = \frac{|p|^2}{2m} + \bar{f}(I_0, x) \tag{2.4}$$

with initial data corresponding to the above-considered asymptotic state.

(ii) Compute the change ΔI of the action by

$$\Delta I = \int_{-\infty}^{\infty} \frac{\partial f}{\partial \varphi}(I_0, \varphi(t), \hat{x}(t))\, dt \tag{2.5}$$

and then compute the corresponding energy exchange $\Delta E = h(I_0 + \Delta I) - h(I_0)$.

Let us here show the outcome of this approximation scheme in the case of a rotator, i.e., for $h(I)=\frac{1}{2}I^2$, and f independent of I; the case of an oscillator is slightly more delicate, and will be discussed in Section 4. To this purpose, let us consider the Fourier expansion of the potential f:

$$f(x, \varphi)=\sum_{k\in\mathbb{Z}} \mathscr{F}_k(x)\, e^{ik\varphi} \tag{2.6}$$

so that

$$\frac{\partial f}{\partial \varphi}=i\sum_{k\in\mathbb{Z}} k\mathscr{F}_k(x)\, e^{ik\varphi} \tag{2.7}$$

From (2.5) one immediately gets

$$\Delta I=\sum_{k\in\mathbb{Z}} \mathscr{I}_k e^{ik\varphi_0}$$

with

$$\mathscr{I}_k=-ik\int_{-\infty}^{\infty} \mathscr{F}_k(\hat{x}(t))\, e^{ik\omega t}\, dt \tag{2.8}$$

By standard arguments (shift of the integration path) one has then

$$\mathscr{I}_0=0, \qquad |\mathscr{I}_k|\leqslant C_k e^{-|k|\,\tau_k\omega} \qquad \text{for} \quad k\neq 0 \tag{2.9}$$

with suitable $C_k>0$, τ_k being the width of the analyticity strip of $\mathscr{F}_k(\hat{x}(t))$. In fact, unless the relevant singularities are simple poles, the "constants" C_k in general depend on ω; the dependence, however, is much weaker than expotential, so in the following this possibility will be neglected. Moreover, in typical cases, one has $\tau_k=\tau$ independent of k, so that, for large ω, the first Fourier component dominates. One has then

$$\Delta I\simeq \mathrm{Re}(\mathscr{I}_1 e^{i\varphi_0})=C_1 e^{-\tau\omega}\cos(\varphi_0-\Phi)$$

with suitable phase Φ. Now, the relation between ΔI and the energy exchange ΔE is, in our case,

$$\Delta E=\omega\,\Delta I+\tfrac{1}{2}(\Delta I)^2 \tag{2.10}$$

If one considers only the above leading term, one then gets

$$\Delta E\simeq \omega C_1 e^{-\tau\omega}\cos(\varphi_0-\Phi) \tag{2.11}$$

More in detail, one can introduce the Fourier decomposition of ΔE,

$$\Delta E=\sum_{k\in\mathbb{Z}} \mathscr{E}_k e^{ik\varphi_0}$$

From (2.9) and (2.11) one then gets different exponential laws for the different Fourier components, namely

$$|\mathscr{E}_0| \leqslant D_0 e^{-2\tau\omega}, \qquad |\mathscr{E}_k| \leqslant \omega D_k e^{-|k|\,\tau\omega} \qquad \text{for} \quad k \neq 0 \tag{2.12}$$

with suitable constants D_k.

The similarity of these results with (1.5) is evident, the only difference being, in (1.5), the absence of higher Fourier components; some further comments on this point are deferred to Section 4. In Section 3 we shall instead perform a quite critical numerical test of these heuristic analytic results, by comparing them with rather accurate numerical results.

3. NUMERICAL RESULTS FOR THE ROTATOR

We study here numerically a particular Hamiltonian system describing the scattering of a rotator by a smooth potential well in one dimension; the Hamiltonian has the form

$$H(I, \varphi, p, x) = \frac{I^2}{2ma^2} + \frac{p^2}{2m} + V(r), \qquad r = x - a\cos\varphi$$

a is a constant (which represents essentially the diameter of the rotator). A system of this form was already considered in ref. 13, which here we partially follow. In a first series of experiments, we consider the particular potential

$$V(r) = V_0 \frac{e^{-r/d}}{r/d} \tag{3.1}$$

We took $a = d/10$, and used m, d, and V_0, respectively, as units of mass, length, and energy.

In each elementary experiment we fix initial data I_0, φ_0, p_0, x_0 with very large x_0 in order for the interaction be negligible; a typical choice is $x_0 = 70d$.[5] Notice that in these conditions I_0 and p_0 practically coincide with the asymptotic quantities introduced in the previous section, and in particular one has $\omega = I_0/(ma^2)$, while φ_0 differs from the asymptotic value for an irrelevant constant. We stop the run when we have again $x = x_0$, and measure the energy exchange ΔE between the translational and the rotational degrees of freedom due to collision; having fixed x_0, ΔE turns out to be a function of I_0, p_0, and φ_0.

[5] For such a value, the interaction is negligible even in quadruple precision (32 decimal digits).

In order to determine the Fourier components $\mathscr{E}_k$ and verify the exponential laws (2.11), (2.12), we compute ΔE for "many" values of φ_0 (we shall be more precise on this point later) at fixed p_0 and ω; then we repeat the cycle of computations for different values of ω at fixed p_0, and finally we repeat the whole set of computations for different values of p_0.

The φ dependence of ΔE at fixed $\omega = 120$ and $p_0 = \sqrt{2}$, i.e., initial translational energy $E_0^x = 1$, is shown in Fig. 1; it is quite evident that, in agreement with the theoretical analysis of the previous section, the first Fourier component actually dominates. Figure 2 reports instead the Fourier coefficients $|\mathscr{E}_k|$, $k = 0, 1, 2, 3$, as functions of ω at fixed $E_0^x = 1$. It is quite clear that, for not too small ω, the data are nicely arranged on straight lines, corresponding to exponential laws of the form

$$|\mathscr{E}_k| = C_k e^{-\lambda_k \omega} \tag{3.2}$$

Notice that one is able to follow the exponential laws over a quite wide range, namely for $|\mathscr{E}_k|$, say, between 10^{-3} and 10^{-30} (*i.e., for 27 orders of magnitude*; see later for comments). According to (2.12), one expects the coefficients λ_k be related to the width τ of the analyticity strip of $\hat{x}$, by

$$\lambda_0 = 2\tau, \qquad \lambda_k = k\tau \qquad \text{for} \quad k \neq 0 \tag{3.3}$$

The quantity τ is computed as follows: quite in general, one has[4]

$$\tau = \left| \operatorname{Im} \int_{x_1}^{x_2} \frac{dx}{\{2[E_0^x - \bar{V}(x)]\}^{1/2}} \right| \tag{3.4}$$

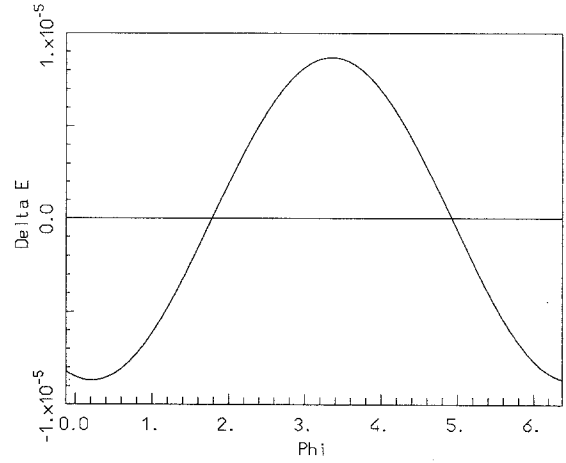

Fig. 1. The energy exchange between rotational and translational degrees of freedom, due to the collision, as a function of the initial phase φ of the rotator.

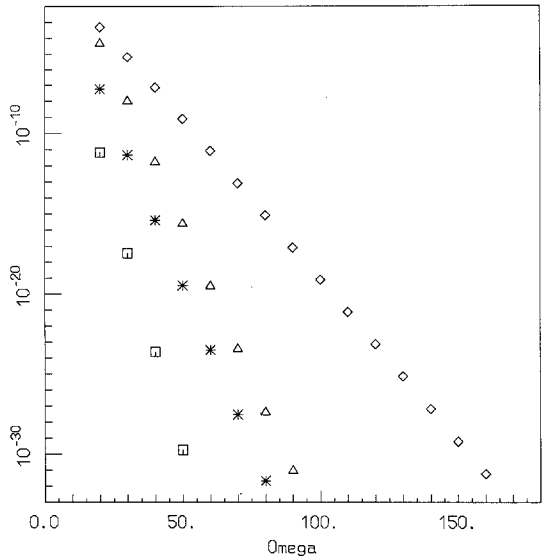

Fig. 2. The amplitude of the Fourier components $|\mathscr{E}_0|$ (triangles), $|\mathscr{E}_1|$ (diamonds), $|\mathscr{E}_2|$ (stars) and $|\mathscr{E}_3|$ (squares), as function of frequency ω, for fixed initial kinetic energy $E_0^x = 1$. The data refer to the potential (3.1).

where $\bar{V}$ is the average of V on the angle φ, while $x_1 = x_1(E_0^x)$ is the turning point of the free motion $\hat{x}(t)$, and x_2 is the location of the relevant singularity of $\bar{V}$ (i.e., the one giving the lowest value of the integral); in the problem at hand, it is not difficult to recognize that one has $x_2 = a$. The integral is easily computed numerically for each given E_0^x; for the above considered value $E_0^x = 1$ one finds $\tau = 0.4709$. At the same time, by a best fit of the last data of Fig. 2 one easily computes the coefficients λ_k; as a result, one gets

$$\lambda_0/\tau = 1.92, \qquad \lambda_1/\tau = 0.988, \qquad \lambda_2/\tau = 1.98, \qquad \lambda_3/\tau = 2.99$$

in good agreement with the theoretical expectation (see, however, the discussion at the end of this section).

Quite similar results are found for different values of E_0^x. In particular, in agreement with the Landau–Teller approximation, the slope λ_1 practically coincides in any case with τ; this can be seen in Table I, where these quantities are reported for three different values of E_0^x.

The possibility of computing energy exchanges as small as those appearing in Fig. 2 may be surprising, namely one can wonder whether such precision is *a priori* compatible with the truncation errors of the numerical

Table I. A Comparison between the Coefficient λ_1 Appearing in the Exponential Law and the Width of the Analyticity Strip τ, at Different Values of E_0^x[a]

E_0^x	λ_1	τ	λ_1/τ
1	0.4656	0.4709	0.9887
2	0.2091	0.2123	0.9849
6	0.0419	0.0427	0.9812

[a] The interaction potential is given by (3.1).

algorithm.[6] We cannot enter here into this delicate question, which is treated in detail in ref. 12. As there explained, the essential point is on one hand the use of a symplectic integration scheme (we used the simplest one, namely the so-called leapfrog algorithm), and on the other hand the fact that, due to the decay of the potential at infinity, asymptotically the algorithm is exact. As a check of consistency, one can make the usual test on the conservation of the total energy; in our conditions, the relative error in the energy conservation at the end of each run never exceeds 10^{-31}. In ref. 12 one can find a wide theoretical discussion of this problem, which is there rigorously studied in the framework of perturbation theory. The essentials of the question, with more emphasis on numerical details, can be found in the already quoted ref. 13, Section 4, where the possibility of very accurate computations of energy exchanges in scattering problems was first recognized (we used here exactly the same numerical method).

Let us then come to the problem of the computation of the Fourier components $\mathscr{E}_k$. We proceeded as follows: we measured the energy exchange ΔE at fixed p_0 and I_0 for N equally spaced initial phases $2\pi l/N$, $l=0,\ldots, N-1$, and then computed the quantity

$$\hat{\mathscr{E}}_k = (1/N) \sum_{l=0}^{N-1} \Delta E(2\pi l/N)\, e^{-2i\pi kl/N} \tag{3.5}$$

For large N, $\hat{\mathscr{E}}_k$ is expected to be a good approximation of $\mathscr{E}_k$. One could imagine that, to reach the precision exhibited in Fig. 2, very large values of N are necessary; in particular, it may appear that the computation of higher harmonics is more difficult for large ω, when they are relatively small. On the contrary, precisely for large ω the value of N turns out to be fairly irrelevant: for example, using $N=256$ or 16 or even 8 gives

[6] Roundoff errors are less important, in particular, if one works (as we did) in quadruple precision, with at least 32 significant digits.

practically identical results. This fact is easily explained as follows: one easily checks that one has

$$\frac{1}{N}\sum_{l=0}^{N-1} e^{-2i\pi kl/N} e^{-2i\pi k'l/N} = \begin{cases} 1 & \text{for } k' = k \bmod N \\ 0 & \text{otherwise} \end{cases}$$

as a consequence, from (3.5) one immediately gets

$$\hat{\mathscr{E}}_k = \sum_{j \in \mathbb{Z}} \mathscr{E}_{k+jN}$$

In our case, the amplitude of the Fourier components decreases so rapidly with k that even for relatively small N, $\hat{\mathscr{E}}_k$ almost coincides with $\mathscr{E}_k$. Practically, in most computations, we used $N=8$, and also, as a check, $N=16$; only in some cases, as a further check, did we use $N=256$. One could see that to compute reliably the first harmonic $\mathscr{E}_1$, even $N=3$ turns out to be sufficient.

The whole sequence of numerical experiments has been repeated for different choices of the interaction potential V, with similar results. For example, Fig. 3 shows the coefficients $|\mathscr{E}_k|$ vs. ω for an interaction potential with an attractive part, namely

$$V(r) = V_0 \left[\frac{1}{2}\left(\frac{d}{r}\right)^2 - \frac{d}{r} \right] e^{-r/d} \tag{3.6}$$

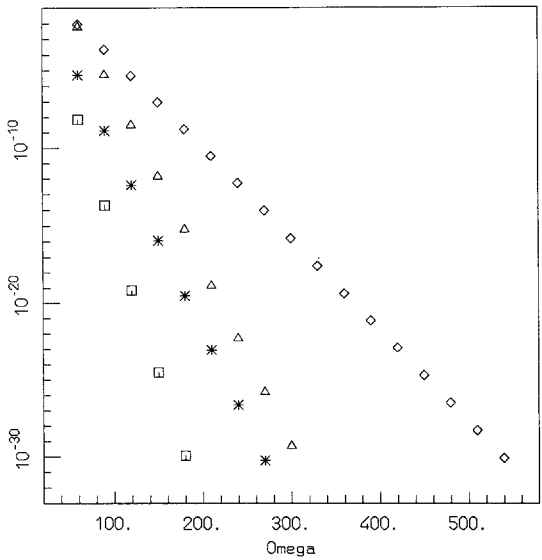

Fig. 3. The same as Fig. 2, for the potential (3.6).

with r being as in (3.1). The figure refers to $E_0^x = 1$ in natural units; for this value of energy, in good agreement with (2.12), one finds

$$\lambda_0/\tau = 1.92,\ \lambda_1/\tau = 0.986,\ \lambda_2/\tau = 1.97,\ \lambda_3/\tau = 2.96$$

The agreement between λ_1 and τ is also good for different values of energy, as shown in Table II.

Similar results, not reported here, have been found for other choices of V, in particular for the potential

$$f(r) = V_0 \frac{e^{-(r/d)^2}}{r/d}$$

considered in the already quoted ref. 13.

As remarked in the Introduction, the heart of the Landau–Teller approximation is the use of the approximate solution $\hat{x}(t)$ in place of the true solution $x(t)$ to compute the width of the analyticity strip τ; correspondingly, the essential result of this section is the coincidence of τ and λ_1. As we have seen, the agreement extends to all Fourier coefficients besides the leading one: this fact is remarkable, but should be taken with some care, and in particular, the situation is not really satisfactory for the average $\mathscr{E}_0$. Indeed, from (2.10), one immediately deduces

$$\mathscr{E}_0 = \omega \mathscr{I}_0 + \sum_{k \geqslant 0} \mathscr{I}_k \mathscr{I}_{-k} \tag{3.7}$$

and the exponential law $\mathscr{E}_0 \sim e^{-2\tau\omega}$ is due to the fact that, according to (2.8), $\mathscr{I}_0$ vanishes, so that the dominant contribution in (3.7) is $|\mathscr{I}_1|^2$. On the contrary, as one could see, numerical computations show that $\mathscr{I}_0$ does not vanish, and, moreover, it gives the dominant contribution to $\mathscr{E}_0$; for this reason, we cannot really say that the Landau–Teller approximation completely explains the exponential law for the average. By the way, one could see that a similar problem also arises for the original version of the approximation, sketched in the Introduction. Let us also notice that (in

Table II. The Same as Table I, for the Interaction Potential (3.6)

E_0^x	λ_1	τ	λ_1/τ
1	0.1375	0.1394	0.9863
2	0.0890	0.0903	0.9856
3	0.0662	0.0676	0.9792

both versions of the approximation) the average of ΔE turns out to be positive definite (i.e., the internal rotational or vibrational energy increases), and this is hardly believable. We are not able to explain why, in spite of these problems, the results for the average and the higher-order harmonics follow so closely the theoretical expectation.

4. RESULTS FOR THE OSCILLATOR

We consider here a Hamiltonian system of the form

$$H(x, y, p_x, p_y) = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2} y^2 + V(r), \qquad r = x - y \tag{4.1}$$

namely a generalization of (1.2); having in mind a scattering problem, one assumes $V(r) \to 0$ for $r \to +\infty$. After the introduction of the usual action–angle variables for the oscillator, one gets (using the same notation H for the Hamiltonian)

$$H(I, \varphi, p_x, x) = \omega I + p_x^2/2m + V(r), \qquad r = x - (2I/m\omega)^{1/2} \sin \varphi \tag{4.2}$$

Let us remark that the use of action–angle variables is very important, not only to apply the theoretical analysis outlined in Section 2, but also to perform accurate numerical integration. Indeed, the use of these variables is necessary to construct a symplectic integration scheme which is asymptotically exact; as remarked in the previous section, this is an essential requirement to reach the high precision we need in the computation of the energy exchanges. The algorithm we used, following ref. 14, is a natural generalization of the leapfrog algorithm, and is implicitly defined by the generating function

$$S(I', \varphi, p_x', x) = I'\varphi + p_x' + \varepsilon H(I', \varphi, p_x', x)$$

ε is the time step.

We made the choice $V(r) = (V_0 d/r)\, e^{-r/d}$ and performed a sequence of numerical experiments similar to the one described in the previous section; more precisely, having fixed $x_0 \gg d$, we computed the energy exchange ΔE as a function of the initial translational energy $E_0^x = p_0^2/2m$, of the vibrational energy $E_0^y = \omega I_0$, of the initial phase φ_0, and of the frequency ω. Figure 4, which is the analog of Figs. 2 and 3, shows the behavior of the first Fourier harmonics $\mathscr{E}_k$ of ΔE as functions of ω at fixed $E_0^x = 2$ and $E_0^y = 1$ (in natural units, as in the previous section). Exactly as for the rotator, one finds exponential laws of the form (3.2).

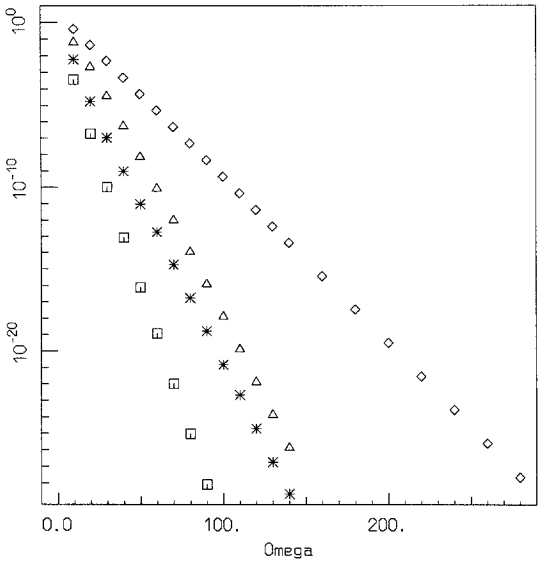

Fig. 4. The same as Fig. 2 and Fig. 3, for the oscillator.

Concerning the theoretical interpretation, there is a minor variant with respect to the case of the rotator, due to the fact that the averaged interaction potential $\bar{f}$ introduced in (2.4) now depends parametrically on ω; more precisely, for our Hamiltonian (4.2), $\bar{f}$ turns out to depend on the ratio $\alpha = (E_0^y)^{1/2}/\omega$. As a consequence (recalling that for the oscillator one has simply $\Delta E = \omega \Delta I$), one finds for the Fourier components of ΔE estimates of the form

$$\mathscr{E}_0 = 0, \qquad |\mathscr{E}_k| \leqslant D_k e^{-|k|\,\tau(\alpha)\omega} \qquad \text{for} \quad k \neq 0 \tag{4.3}$$

which differ from a pure exponential because τ now depends on α and thus on ω. However, the exponential estimate does not disappear, since for large ω, at fixed initial energy E_0^y, τ tends to a constant τ_0; this can be seen by an inspection of the integral expression of τ, similar to (3.4). One could also see that τ_0 coincides with the corresponding constant in the original Rapp implementation of the Landau–Teller method. The behavior of τ as a function of ω at fixed $E_0^y = 1$ is reported in Fig. 5 (solid line); one can see that even for not too large values of ω, τ is practically constant.

From Fig. 4 one easily deduces, by a best fit on the last data, the asymptotic values of the slope λ_k for $k = 0, 1, 2, 3$; as a result one finds

$$\lambda_0/\tau_0 = 1.944, \qquad \lambda_1/\tau_0 = 0.993, \qquad \lambda_2/\tau_0 = 1.980, \qquad \lambda_3/\tau_0 = 2.971$$

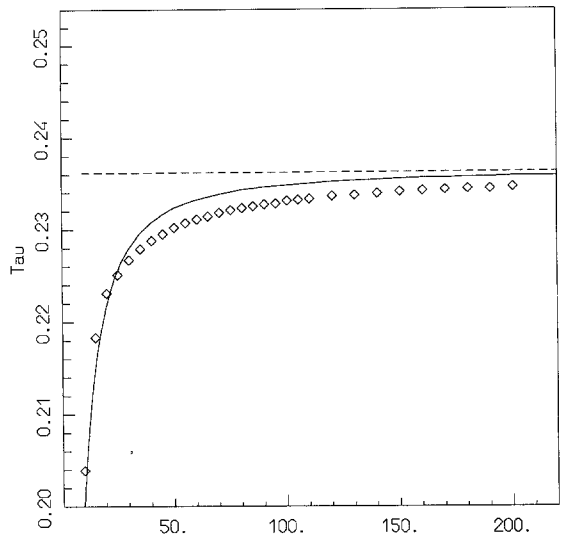

Fig. 5. The value of τ given by (3.4) as function of ω (solid line); the asymptotic value τ_0 for $\omega \to \infty$ (dashed line); the slope of the curve $\log |\mathscr{E}_1|$ as function of ω (diamonds).

As one can see, the agreement with (4.3) is satisfactory, with the exception of the average $\mathscr{E}_0$, for which one could repeat the considerations made at the end of the previous section. By the way, besides the asymptotic slope, one can also evaluate each λ_k as a function of ω; this was done for the first Fourier component $\mathscr{E}_1$, and the result is presented in Fig. 5 (diamonds). As a matter of fact, λ_1 appears to follow rather closely τ, even before the asymptotic regime.

The asymptotic values of λ_1 and τ at different values of E_0^x for fixed $E_0^y = 1$ are reported in Table III. We also made computations with other choices of the interaction potential, with essentially similar results.

Table III. The Same as Tables I and II, for the Oscillator with the Hamiltonian (4.1)

E_0^x	λ_1	τ_0	λ_1/τ_0
1	0.4936	0.4964	0.994
2	0.2347	0.2363	0.993
3	0.1460	0.1469	0.994

5. THE LARGE-ω BEHAVIOR OF "TRUE" SINGULARITIES

In the previous sections, in agreement with the fundamental idea of the Landau–Teller approximation, we made reference to the free motion $\hat{x}(t)$, namely the solution of the averaged equation (2.4), and in particular to the distance τ of the relevant singularity from the real axis. In this section we compare τ with the corresponding quantity τ^*, relative to the true solution $x(t)$. One could expect that τ is close to τ^*, at least for large ω (see the short discussion in the Introduction); in fact, as shown in the already quoted ref. 11, this is the case for the oscillator if the initial energy E_0^y vanishes. Instead, as we shall see, the situation is apparently totally different if one considers the rotator or the oscillator at nonvanishing E_0^y: indeed, not does only τ^* turn out to be quite different from τ, but apparently it goes to zero for large ω.

The value of τ^* can be computed numerically in the following way: denote by $t = s + i\sigma$ the complex time variable; let $t_0 = s_0$ be the (real) initial time, with $x(t_0) \gg d$, and let $t_1 = s_1$ be the corresponding final time, much after the collision. Consider, then, in addition to the usual real integration path from t_0 to t_1, a complex path with the same ends, composed of the three segments $(t_0, s_0 + i\sigma)$, $(s_0 + i\sigma, s_1 + i\sigma)$, and $(s_1 + i\sigma, t_1)$. If $\sigma < \tau^*$, then the change of any dynamical variable along the two paths

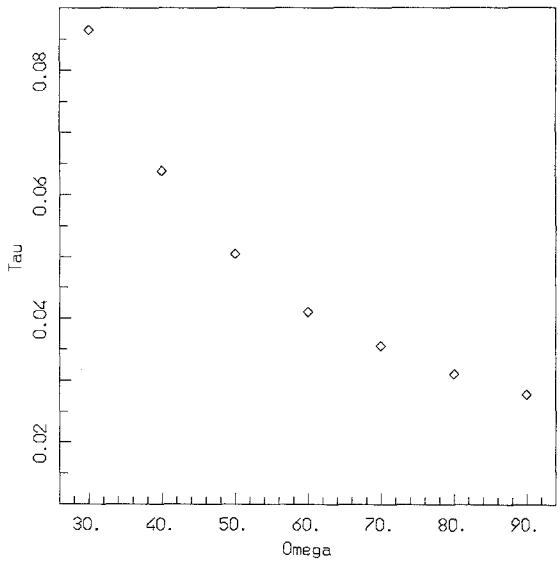

Fig. 6. The analyticity strip τ^*, relative to the true motion $x(t)$, as a function of ω, for a rotator with interaction potential (3.1).

must coincide. We found it convenient to use as a test variable the energy exchange ΔE itself, and observed that ΔE as function of σ for fixed initial data is practically a step function: it remains constant and very close to zero (for large ω) for σ up to a rather well-defined value τ^* and then jumps to a value of order one. Other dynamical variables present a similar discontinuous behavior. On the contrary, the total energy is found to be practically insensitive to the crossing of the singularity, as it should be, since the energy in principle is independent of t (energy in particular is always well conserved). In our opinion, this is a somehow critical test on the reliability of the above procedure to compute τ^*.

The value of τ^* depends on the initial data, in particular on ω; a typical result is illustrated in Fig. 6, where τ^* is plotted versus ω for the case of the rotator, with interaction potential (3.1), at $E_0^x = 1$. The difference between τ^* and τ, as reported in Table I, is striking. Similar results were also found for other potentials as well as for the oscillator in the case of nonvanishing E_0^y. The whole situation, in our opinion, is somehow paradoxical; a short comment on this point is deferred to the Conclusions.

6. CONCLUSION

The Landau–Teller heuristic approach to adiabatic invariants has been critically revisited and applied to particular models, describing elementary scattering processes of fast oscillators or rotators. The essence of the approach is the interpretation of the coefficient λ of ω in the exponential laws as the width of the analyticity strip of the solutions of the system extended to complex times; the heart of the approximation is replacing the true value τ^* of the analyticity width with the corresponding value τ of a drastically simplified scattering problem, namely a problem in which the internal degree of freedom is suppressed, either by putting to zero its amplitude, as in the original version of the approximation, or by suitably averaging on a phase, as we did in our action–angle reformulation of the approximation.

Quite accurate numerical experiments have been performed to test the reliability of the Landau–Teller approach. The results, as we have seen, are quite embarrassing; indeed, the approximation seems to works *excellently*, both qualitatively and quantitatively (even in the details, namely concerning the behavior of higher Fourier components) if one makes reference to the "approximate" value τ; on the contrary, it completely fails if one refers to the "true" quantity τ^* (the only exception is the case considered in ref. 11, namely the oscillator at zero initial energy, for which, asymptotically for large ω, τ and τ^* turn out to coincide). Of course, numerical tests

are affected by errors: however, as we have seen, there are good theoretical reasons to believe that, in the problem at hand, numerical errors are negligible; moreover (as is perhaps the best accuracy test) the overall coherence and evidence of numerical results is, in our opinion, particularly sharp.

It is not so easy to interpret such results. However, the failure of the approach if based on the behavior of the true solution $x(t)$ is not totally unexpected if one recalls some basic facts of classical perturbation theory. The idea is roughly as follows: as is well known, in classical perturbation theory one constructs small canonical changes of variables which give the Hamiltonian a suitable normal form; with reference, say, to the oscillator Hamiltonian (4.2), one introduces a canonical transformation

$$(I, \varphi, p, x) = \mathscr{C}(I', \varphi', p', x'; \omega) \tag{6.1}$$

near to the identity for large ω, such that the transformed Hamiltonian $H' = H \circ \mathscr{C}$ is φ' independent up to an exponentially small remainder: say,

$$H' = \omega I' + \frac{p'^2}{2m} + V(x') + \omega^{-1} g(I', p', x'; \omega) + \omega^{-1} e^{-\omega/\omega^*} f'(I', \varphi', p', x'; \omega) \tag{6.2}$$

with suitable ω^*; both H' and the canonical transformation $\mathscr{C}$ turn out to be analytic in a convenient complex domain.

To make clear the source of the difficulties, and understand in particular why for large ω the singularities of $x(t)$ get closer to the real axis, let us forget the small remainder in (6.2), whose role at this point is not essential. The behavior of the normalized variables I', φ', p', and x' is then trivial: indeed, one has $I'(t) = I'_0$, $\varphi'(t) \simeq \varphi'_0 + \omega t$, while p', x' practically move as in a free collision; in particular, $x'(t)$ and $p'(t)$ turn out to be analytic for t in some complex strip whose width is independent of ω. The situation, however, drastically changes if one looks at the original variables $x(t)$ and $p(t)$: indeed, assume, to be definite, that the canonical transformation (6.1) is analytic as a function of the angle φ' in a strip $|\mathrm{Im}\, \varphi'| < \rho$; clearly, for $|\mathrm{Im}\, t| > \rho/\omega$, $\varphi'(t)$ escapes the analyticity domain, and correspondingly, all of the original variables are expected to become singular.[7] The presence of the exponentially small remainder cannot change substantially such a picture; in particular, one should expect that for large ω the analyticity strip of $x(t)$ is roughly proportional to ω^{-1}, as we find in our numerical computations.

From this heuristic discussion, it appears clearly that on one hand the difficulty is unavoidable, and on the other hand it is somehow spurious,

[7] This is not in contrast with the results of ref. 11, since for vanishing initial action, $x(t)$ and $p(t)$ turn out to be almost independent of φ'.

being related, so to speak, to the use of "wrong" variables to describe the motion. It is quite clear, in our opinion, that the approximate motion $\hat{x}(t)$ leads to good results, not because it is close to $x(t)$, but rather because it is close, from the point of view of the analytic structure, to the normalized motion $x'(t)$, so that the above spurious difficulty is absent. We plan to analyze this delicate question in the near future, and more generally, to study more deeply the relation between the Landau–Teller approach and the methods of classical perturbation theory.

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