Accuracy loss of action invariance in adiabatic change of a one-freedom Hamiltonian

1986 J. Phys. A: Math. Gen. 19 L1067

(http://iopscience.iop.org/0305-4470/19/17/004)

J. Phys. A: Math. Gen. 19 (1986) L1067-L1072. Printed in Great Britain

LETTER TO THE EDITOR

Accuracy loss of action invariance in adiabatic change of a one-freedom Hamiltonian

J H Hannay

H H Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK

Received 4 August 1986

Abstract. The action in a one-freedom Hamiltonian system is well known to be invariant under adiabatic change of the Hamiltonian with very small error, provided the frequency of the motion does not vanish. But the frequency *can* generically vanish: a potential barrier can pass through the energy of the particle. The error incurred in this case has a universal form which is calculated.

If a particle is moving in a one-dimensional potential well it follows a contour of constant energy in phase space. If the potential is changed infinitely slowly to a new one, the contours change shape. But since work is done on the particle it does not, finally, follow that contour with the same energy as initially, but rather that with the same area, or action, as initially. This is the well known adiabatic invariant of integrable systems (Arnold 1978) and it continues to hold approximately provided the timescale of the change is much greater than the period of oscillation. In fact the error is exponentially small in this ratio if the change is a smooth one (Landau and Lifshitz 1969).

Loss of accuracy may be expected, though, if the change in the potential is such as to take the frequency of oscillation to zero. This happens generically when a potential barrier passes through the energy of the particle. The process and the consequent loss of accuracy incurred is described below.

Figure 1 shows the instantaneous action S of a particle (that is the area of the Hamiltonian contour it lies on) as the potential it is moving in is very slowly changed. The potential is a symmetric one-dimensional double well whose central barrier is slowly lowered so that the particle escapes from the right-hand well to move in both wells. In phase space the separatrix of the Hamiltonian (the contour through the barrier peak) shrinks through the orbit of the particle. Its action, for one half, not both, is shown by a broken line. The action of the particle makes its largest jump at the transition through the separatrix, where it collects the area of the left-hand lobe, and is therefore doubled, approximately. The question is, how approximately (exact doubling not being counted as accuracy lost).

Both before and after the transition the motion divides into alternating 'sweeps' and 'creeps'. The sweeps are *fast* traversals of one or other lobe of the separatrix with the orbit hugging it closely. The creeps are *slow* passages through the central hyperbolic region, corresponding to reflection from, or passage over, the barrier. During the creeps the action of the particle parallels that of the separatrix, because its contour keeps hugging the separatrix (except in the immediate hyperbolic neighbourhood).

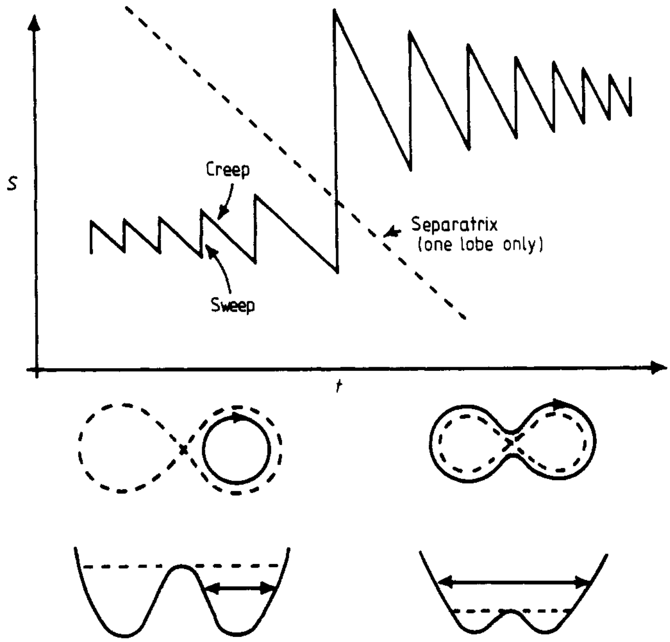

Figure 1. Instantaneous action S of a particle as the potential it moves in is slowly changed.

The creep lines on the graph are twice as steep after the transition as before because the contour then encloses both of the separatrix lobes. During the sweeps the action changes for another reason (they are too fast for the separatrix action to change appreciably). Work is done on the particle so that it returns to the hyperbolic region for its next creep on a higher energy contour with, therefore, a different area (figure 2).

The relation between the energy and the area takes a universal form when, as we assume throughout, the energy is close enough to the barrier top energy. In fact it is

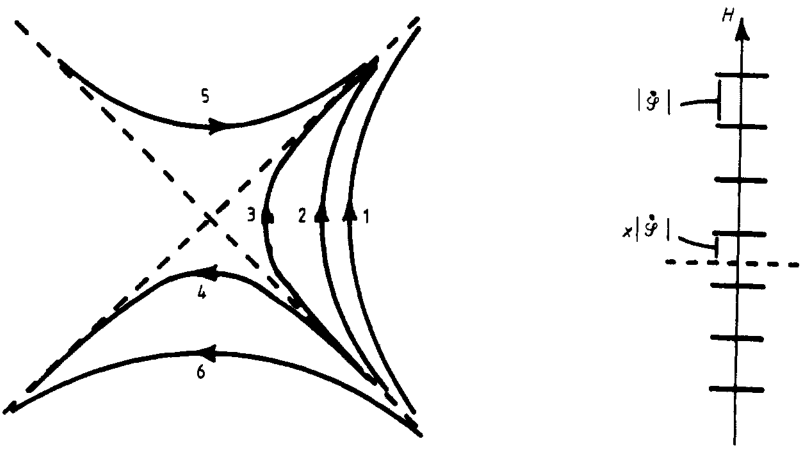

Figure 2. Successive creep contours and their energies.

convenient to take the latter as the zero of energy so that the wells are rising rather than the barrier falling. Then the energy H of a particle is *constant* during a creep and the difference between its contour area and the separatrix area can be written

$$A = -\tau H(\ln|H|/h - 1) \tag{1}$$

where τ is the characteristic time of the hyperbolic point (a local feature) and h is a constant determined by the gradient of the Hamiltonian around the entire lobe (a global feature).

The duration of a creep is the derivative of A with respect to H:

$$-\tau \ln|H|/h \tag{2}$$

which is large close to the transition when $|H|$ is small and diminishes as $|H|$ grows. ($|H|$ is necessarily much less than h for the formula to be applicable.)

Although the particle's action continues to oscillate long after (and long before) the transition, its mean final value $S_{\rm f}$ is well defined and expressible in terms of its mean initial value $S_{\rm i}$ as follows. Pick a particular 'initial' sweep i, long before the transition, and a 'final' one f long after. Denote the separatrix area (one lobe thereof) at these instants by $\mathcal{S}_i$ and $\mathcal{S}_f$ and its constant rate of change by $\dot{\mathcal{S}}$ (negative in value). With A_{i-} and A_{i+} as the area difference (1) during the creeps immediately before and after sweep i, and similarly for A_{f-} and A_{f+}, we have

$$\begin{aligned} S_{\rm f} &= 2\mathcal{S}_f + \tfrac{1}{2}(A_{f+} + A_{f-}) \\ &= 2\mathcal{S}_i + 2\dot{\mathcal{S}}\textstyle\sum - \tau \ln|H|/h + \tfrac{1}{2}(A_{f+} + A_{f-}) \\ &= 2S_i + 2\dot{\mathcal{S}}\textstyle\sum - \tau \ln|H|/h + \tfrac{1}{2}(A_{f+} + A_{f-}) - (A_{i+} + A_{i-}) \end{aligned} \tag{3}$$

where the summation runs over all creep energies between sweep i and sweep f.

The final fact that allows explicit evaluation of $S_{\rm f}$ is that the work done on the particle in each sweep is the *same*, its value being simply $-\dot{\mathcal{S}}$. (This follows from the equality of the integrals $\int \partial H/\partial t \, {\rm d}t$ and $\int \partial S/\partial t \, {\rm d}\theta/2\pi$ around the lobe, θ being the angle variable.) So the creep energies are an equally spaced ladder of steps which the particle climbs (figure 2):

$$H = |\dot{S}|(n + x) \qquad \text{for integer } n \tag{4}$$

where the only freedom is the overall shift x. This is the 'random' variable associated with the exact phase of oscillation that the particle has at the critical moment. If i and f are sufficiently early and late respectively then x is uniformly distributed on the range 0-1.

Using the following identity (the derivative of the identity is well known and the integral of each side from $x = 0$-1 is equal to zero as $N \to \infty$):

$$\begin{aligned} &\lim_{N\to\infty} \sum_0^N \ln(n+x) - \tfrac{1}{2}\{(N+x)[\ln(N+x) - 1] + (N+x+1)[\ln(N+x+1) - 1]\} \\ &\qquad = -\ln \Gamma(x)/\sqrt{2\pi} \end{aligned} \tag{5}$$

we obtain, by separating the sum in (3) into a pre- and post-transition sum and substituting for the A from (1),

$$\begin{aligned} S_{\rm f} &= 2S_{\rm i} - 2|\dot{\mathcal{S}}|\tau[\ln(\Gamma(x)/\sqrt{2\pi}) - (\tfrac{1}{2} - x)\ln|\dot{\mathcal{S}}|/h] \\ &\qquad - 2|\dot{\mathcal{S}}|\tau[\ln(\Gamma(1-x)/\sqrt{2\pi}) - (-\tfrac{1}{2} + x)\ln|\dot{\mathcal{S}}|/h] \\ &= 2S_{\rm i} + 2|\dot{\mathcal{S}}|\tau \ln(2\sin \pi x) \qquad \text{(independent of the constant } h\text{).} \end{aligned} \tag{6}$$

Since x is distributed on the interval 0-1, the distribution (figure 3) of the final action S_f is straightforwardly shown to be

$$P(S_f)=\frac{1}{\pi|\dot{\mathscr{S}}|\tau}(\exp(-\Delta S/|\dot{\mathscr{S}}|\tau)-1)^{-1/2} \tag{7}$$

where

$$\Delta S=S_f-2S_i-\pi|\dot{\mathscr{S}}|\tau \qquad (\Delta S<0). \tag{8}$$

(The average value of ΔS is, from (7), $-\pi|\dot{\mathscr{S}}|\tau$, which means the average value of S_f is just $2S_i$ as would be expected.)

For the reverse process of capture of the particle by one side or the other as the wells become deeper, the expressions analogous to (3) are

$$\begin{aligned} S_f &= \mathscr{S}_f+\tfrac{1}{2}(A_{f+}+A_{f-})=\mathscr{S}_i+\dot{\mathscr{S}}\left(\sum\right)+\tfrac{1}{2}(A_{f+}+A_{f-}) \\ &=\tfrac{1}{2}[S_i-\tfrac{1}{2}(A_{i+}+A_{i-})]+\dot{\mathscr{S}}\left(\sum\right)+\tfrac{1}{2}(A_{f+}+A_{f-}) \\ &=\tfrac{1}{2}S_i+\dot{\mathscr{S}}\left(\sum\right)+\tfrac{1}{2}(A_{f+}+A_{f-})-\tfrac{1}{4}(A_{i+}+A_{i-}) \end{aligned} \tag{9}$$

so that the action change is

$$S_f=\tfrac{1}{2}S_i-|\dot{\mathscr{S}}|\tau\ln(2\sin\pi x) \tag{10}$$

and its distribution is

$$P(S_f)=\frac{2}{\pi|\dot{\mathscr{S}}|\tau}(\exp(-\Delta S/|\dot{\mathscr{S}}|\tau)-1)^{-1/2} \tag{11}$$

where

$$\Delta S=S_f-\tfrac{1}{2}S_i+\tfrac{1}{2}\pi|\dot{\mathscr{S}}|\tau \qquad (\Delta S>0). \tag{12}$$

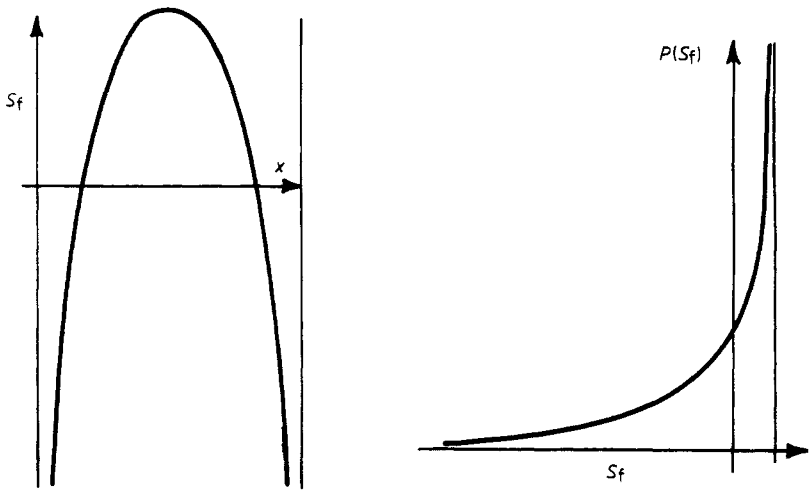

Figure 3. Final action as a function of the 'random' variable x and its consequent distribution.

The generalisation to asymmetric wells is straightforward. The most obvious difference is that the escaping particle collects an action from the left-hand separatrix lobe which has no relation to the right-hand lobe area. Let the area of the left lobe when the right one has an area equal to the initial particle action S_i be $\mathcal{S}_0^l$. Another important difference is that the constant rates of change $\dot{\mathcal{S}}^l$ and $\dot{\mathcal{S}}^r$ need no longer be equal, though both should be considered negative as before. The energy changes during the sweeps after the transition therefore alternate between $-\dot{\mathcal{S}}^r$ and $-\dot{\mathcal{S}}^l$. This alternation shows up in the action graph as alternating large kicks and small ones. Finally the constant h now takes a different value h^l and h^r for left and right lobes. We will use the fact that the area between the separatrix and an exterior contour of energy H is the same as the sum of the two areas between the contours of energy $-H$ and their separatrix lobes. Thus

$$A = -\tau H(\ln |H|/h^r - 1) - \tau H(\ln |H|/h^l - 1) \tag{13}$$

after the transition. The creep duration is the derivative of this divided by two:

$$-\tau \ln(|H|/\sqrt{h^r h^l}). \tag{14}$$

Thus we have

$$\begin{aligned} S_f &= \mathcal{S}_f^r + \mathcal{S}_f^l + \tfrac{1}{2}(A_{f+} + A_{f-}) \\ &= \mathcal{S}_i^r + \mathcal{S}_i^l + (\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l)\left(\sum_{\text{Pre}} -\tau \ln \frac{|H|}{h^r} + \sum_{\text{Post}} -\tau \ln \frac{|H|}{\sqrt{h^r h^l}}\right) + \tfrac{1}{2}(A_{f+} + A_{f-}) \\ &= S_i - \tfrac{1}{2}(A_{i+} + A_{i-}) + \mathcal{S}_0^l - \tfrac{1}{2}(A_{i+} + A_{i-})\dot{\mathcal{S}}^l/\dot{\mathcal{S}}^r + (\dot{\mathcal{S}}^l + \dot{\mathcal{S}}^r)\left(\sum\right) + \tfrac{1}{2}(A_{f+} + A_{f-}) \\ &= S_i + \mathcal{S}_0^l + (1 + \dot{\mathcal{S}}^l/\dot{\mathcal{S}}^r)\left(\dot{\mathcal{S}}^r \sum_{\text{Pre}} -\tau \ln \frac{|H|}{h^r} - \tfrac{1}{2}(A_{i+} + A_{i-})\right) \\ &\quad + \left((\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l) \sum_{\text{Post}} -\tau \ln \frac{|H|}{\sqrt{h^r h^l}} - \tfrac{1}{2}(A_{f+} + A_{f-})\right). \end{aligned} \tag{15}$$

The final step is to split the 'post' sum into two parts corresponding to up creeps (e.g. 5 in figure 2) and down creeps (e.g. 4 and 6 in figure 2), each of which has a uniformly spaced ladder of energies with spacing $|\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l|$. It is easy to check that the term $\tfrac{1}{2}(A_{f+} + A_{f-})$ can be replaced (with vanishing error) by terms for the ups and downs separately. Thus we obtain

$$\begin{aligned} S_f = S_i &+ \mathcal{S}_0^l + (1 + \dot{\mathcal{S}}^l/\dot{\mathcal{S}}^r)|\dot{\mathcal{S}}^r|\tau[\ln \Gamma(x^r)/\sqrt{2\pi} - (\tfrac{1}{2} - x^r) \ln |\dot{\mathcal{S}}^r|/h^r] \\ &+ |\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l|\tau[\ln \Gamma(x^u)/\sqrt{2\pi} - (\tfrac{1}{2} - x^u) \ln |\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l|/(h^r h^l)^{1/2}] \\ &+ |\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l|\tau[\ln \Gamma(x^d)/\sqrt{2\pi} - (\tfrac{1}{2} - x^d) \ln |\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l|/(h^r h^l)^{1/2}] \end{aligned} \tag{16}$$

where x^r, x^u, x^d are the 'phases' of the three energy ladders (figure 4), i.e.

$$\begin{aligned} &\text{up creep energies:} && |\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l|(n + x^u) \\ &\text{down creep energies:} && |\dot{\mathcal{S}}^r + \dot{\mathcal{S}}^l|(n + x^d) \\ &\text{right creep energies:} && -|\dot{\mathcal{S}}^r|(n + x^r). \end{aligned} \tag{17}$$

Between the completion of this letter and its submission, I learned of other simultaneous work on this problem (Tennyson *et al* 1986a, b).

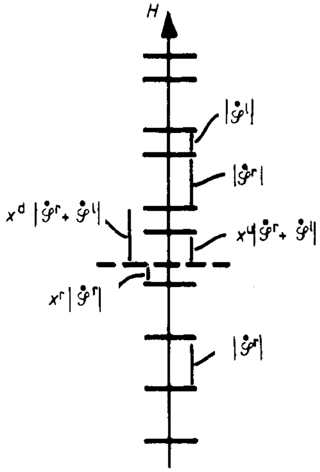

Figure 4. Energy ladder for asymmetric well.

I am grateful to M Robnik for posing this problem and for his work towards solving it.

References

Arnold V I 1978 *Mathematical Methods of Classical Mechanics* (Berlin: Springer)
Landau L D and Lifshitz E M 1969 *Mechanics* (Oxford: Pergamon) 2nd edn
Tennyson J L, Cary J R and Escande D F 1986a *Phys. Rev. Lett.* **56** 2117
—— 1986b *Phys. Rev.* A to be published