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PERIODIC LIBRATIONS AND THEIR EFFECT ON THE QUANTUM ENERGY SPECTRUM*

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Classical Hamiltonian systems with time-reversal symmetry have periodic orbits of two kinds – symmetry pairs (rotations) and self-symmetric orbits (librations). For integrable anharmonic oscillators with two freedoms, almost all of periodic orbits of any period are rotation pairs. However, we show that a KAM-type perturbation alters this balance, such that a finite fraction of the low-period orbits are librations. The generic bifurcations undergone by librations are isomorphic to those of non-symmetric orbits of structurally stable Hamiltonians, with the addition of an extra type of periodic bifurcation. We determine the unfolding of this bifurcation as time-reversal symmetry is broken. The effect of this non-structurally stable bifurcation on the quantum mechanical density of states is also obtained. The present results also hold for systems that are symmetric with respect to general anti-unitary symmetries in quantum mechanics, corresponding to anticanonically reversible Hamiltonian classical systems.

1. Introduction

There are many important Hamiltonian systems that are not *structurally stable*, i.e., they have a peculiar property that can disappear as a result of an arbitrarily small perturbation. An important example is the time-reversal symmetry characteristic of Hamiltonians of the form $\frac{1}{2}\boldsymbol{p}^2 + V(\boldsymbol{q})$, where $\boldsymbol{p}$ and $\boldsymbol{q}$ are the canonical momenta and coordinates in phase space. If the Hamiltonian describes the motion of a charged particle and we add an arbitrarily small magnetic field specified by the vector potential $\epsilon \boldsymbol{A}(\boldsymbol{q})$, the coordinate motion loses the symmetry by which exchanging $\boldsymbol{p}$ for $-\boldsymbol{p}$ is equivalent to exchanging t for $-t$. The time-reversal symmetry is only the most famous example of a wide class of anti-unitary symmetries [1], for instance Robnik and Berry [2] show that a generalized time-reversal invariance may still hold under special conditions, even in the presence of a magnetic field.

The classical limit of these systems belongs to the general class of *reversible systems* [3] with respect to anti-canonical transformations. We show in the appendix how an anti-canonical reversing involution can be reduced by a canonical

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change of coordinates to a simple time-reversal, so we will restrict our discussion to this physically important case.

Birkhoff [4], De Vogelaere [5], Devaney [3] and Greene et al. [6] have discussed the way that reversibility can be an aid in the calculation of periodic orbits. These are the basic ingredients in the celebrated semi-classical sum formula for the density of energy eigenstates [7] in quantum mechanics. However, early attempts to calculate the energy spectrum from the symmetric periodic orbits proved disappointing [8]. We shall discuss below why we should indeed expect that symmetric periodic orbits would be insufficient for this purpose. The more surprising fact that the simpler families of periodic orbits can all turn out to be symmetric will also be explained.

Through any phase point $\boldsymbol{x}=(\boldsymbol{p},\boldsymbol{q})$ there will pass an orbit (usually non-periodic), and there will also be an orbit passing through its symmetry image $(-\boldsymbol{p},\boldsymbol{q})$. If the number of freedoms is greater than one, there is zero probability that both these orbits are the same. The reason is that all points on the orbit will then have this property and it must therefore pass through the plane $\boldsymbol{p}=0$. The orbits crossing this plane fill an $(L+1)$-dimensional manifold within the $2L$-dimensional phase space, so typical orbits do not have this property. This genericity argument holds for both integrable and non-integrable systems.

We refer to self-symmetric periodic orbits as generalized *librations* and symmetry pairs as *rotations* in analogy to the simple pendulum. Among the periodic orbits of any period, almost all are rotation pairs instead of being self-symmetric, in the case of integrable systems discussed in section 2. The situation for fully or partially chaotic systems is less clear, though one may intuitively expect that rotations will dominate over librations just as do general non-symmetric orbits over open self-symmetric orbits. (For canonical, as opposed to anti-canonical symmetries, there can be an identification of symmetric orbits with periodic orbits, as remarked by Gutzwiller [9].) An indication that librations do comprise a negligible proportion of the long-period orbits of a chaotic system is the success of this assumption in explaining universal statistical properties of the quantum energy spectrum [10–12].

Here we draw attention to a surprising exception to this dominance of rotations over librations. For non-integrable (but time-reversal preserving) perturbations of two-dimensional harmonic oscillators, it is mainly periodic *rotations* that are destroyed, whereas periodic *librations* are preserved. (There is no necessary contradiction with the assumption of the previous paragraph, because the overwhelming rotations should be long-period orbits associated with high-order KAM island structure). As the energy and therefore the effect of the anharmonicity is increased, the librations will undergo successive bifurcations, but symmetry will constrain almost all the products of these bifurcations to be again librations. The only exception (among the bifurcations that may generically occur in systems with time-reversal symmetry) is an isochronous (period-1) bifurcation which was added by Rimmer [13, 14] to the list of generical bifurcations occurring in structurally stable systems derived by Meyer [15]. This bifurcation produces a symmetric pair of satellite rotations which coalesce with the central libration.

The analysis of two-dimensional anharmonic oscillators, leading to the result that a pair of librations survive the breakup of a resonant torus under a KAM perturbation is presented in section 2. In section 3 we supply the generating functions for the Poincaré map of Meyer's generic isochronous bifurcation and the symmetric type of Rimmer. We also determine how the bifurcation unfolds into the generic form when the time-reversal symmetry is broken by applying catastrophe theory [16].

Finally we consider the effect of librations on the energy spectrum in section 4. It is shown in ref. [17] that the contribution of bifurcating periodic orbits to the periodic orbits sum is not singular as in the original theory of Gutzwiller [7]. The amplitude of the bifurcating orbit is given directly in terms of the generating function for the Poincaré maps. As recently verified [18] these orbits generate sharp nearly periodic peaks in the density of states. Due to the importance of librations among short-period orbits, it is necessary to add the symmetric bifurcation to those already established for Meyer's generic list. We also derive semiclassical conditions for the cases when bifurcating orbits of systems which nearly have time-reversal symmetry must be treated by using the unfolded generating function for the symmetric bifurcation.

2. Time-symmetric periodic orbits in anharmonic oscillators

Consider a two-freedom system with a classical Hamiltonian of the form

$$H(\boldsymbol{p},\boldsymbol{q}) = \tfrac{1}{2}p_1^2 + \tfrac{1}{2}p_2^2 + V(q_1, q_2), \tag{1}$$

where $V(\boldsymbol{q})$ is a convergent power series whose lowest-order terms are

$$V_2(q_1, q_2) = \tfrac{1}{2}\omega_1^2 q_1^2 + \tfrac{1}{2}\omega_2^2 q_2^2. \tag{2}$$

A canonical change of scale of the $\boldsymbol{p}$ and $\boldsymbol{q}$ axes brings (1) into the standard form

$$H(\boldsymbol{p},\boldsymbol{q}) = \omega_1\left[\tfrac{1}{2}(p_1^2+q_1^2)\right] + \omega_2\left[\tfrac{1}{2}(p_2^2+q_2^2)\right] + \sum_{n\geq 3} V_{n_1 n_2} q_1^{n_1} q_2^{n_2}. \tag{3}$$

The motion is constrained to the *energy shell* defined by the initial conditions $(\boldsymbol{p}_0, \boldsymbol{q}_0)$, that is,

$$H(\boldsymbol{p}(t),\boldsymbol{q}(t)) = H(\boldsymbol{p}_0,\boldsymbol{q}_0) \equiv E. \tag{4}$$

Since the origin is a local minimum of the Hamiltonian, the energy shell for $E = 0$ reduces locally to a single point. For small $E > 0$ all the points in the shell are close to the origin, so the Hamiltonian is dominated by its quadratic terms. In other words, the motion for small E is approximately that of a pair of uncoupled harmonic oscillators for which

$$I_1 = \tfrac{1}{2}(p_1^2 + q_1^2) \quad \text{and} \quad I_2 = \tfrac{1}{2}(p_2^2 + q_2^2) \tag{5}$$

are constants of the motion. In this approximation each orbit lies on a *torus* that projects onto $\boldsymbol{q}$ space as a rectangular box (a Lisajous figure) touching the energy shell as shown in fig. 1a. The orbits for all tori on all the energy shells will be periodic if the frequency ratio ω_1/ω_2 is a rational number. If this ratio is irrational the orbits will be non-periodic, with the exception of the orbits lying on the q_1 or q_2 axes, that is, in the case of degenerate infinitely thin tori.

The effect of the non-harmonic terms in the Hamiltonian become more important as the energy is increased. An improvement on the harmonic approximation is then provided by the *Birkhoff normal form* (see e.g. ref. [19] or [10]). There exist canonical transformations $(\boldsymbol{q}, \boldsymbol{p}) \rightarrow$

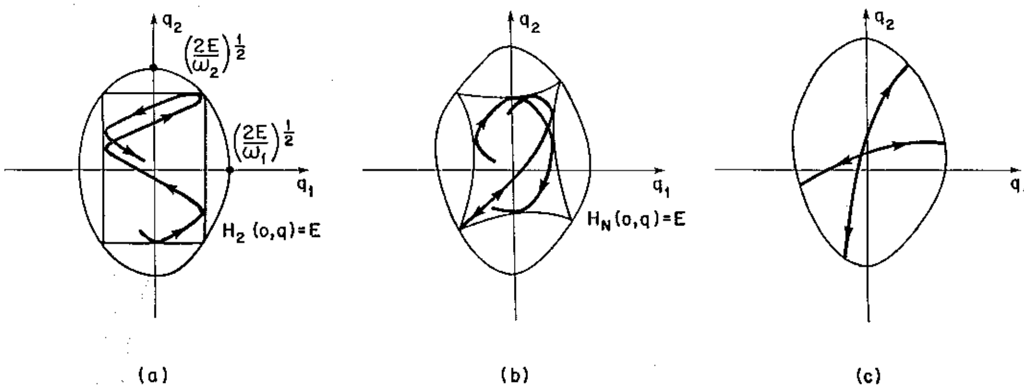


Fig. 1. Projection on $\boldsymbol{q}$ space of a box torus for (a) $H_2(\boldsymbol{q}, \boldsymbol{p})$ and (b) $H_N(\boldsymbol{q}, \boldsymbol{p})$. Infinitely thin tori are shown in (c).

$(\boldsymbol{Q}, \boldsymbol{P})$ that reduce the Hamiltonian to the form

$$H(\boldsymbol{p},\boldsymbol{q}) = H_N\left(\tfrac{1}{2}\left(P_1^2+Q_1^2\right), \tfrac{1}{2}\left(P_2^2+Q_2^2\right)\right) + \sum_{m_1+n_1+m_2+n_2 \geq 2N} P_1^{m_1} Q_1^{n_1} P_2^{m_2} Q_2^{n_2}, \tag{6}$$

where the normalized Hamiltonian H_N is a polynomial of order N in its arguments whose second-order terms coincide with the harmonic terms in (3). The motion generated by H_N is still bound to tori determined by the actions

$$\boldsymbol{I} = \left(\tfrac{1}{2}\left(P_1^2+Q_1^2\right), \tfrac{1}{2}\left(P_2^2+Q_2^2\right)\right).$$

However, the frequencies for the motion on each torus are now specified by

$$\dot{\theta}_1 = \omega_1(\boldsymbol{I}) = \frac{\partial H_N}{\partial I_1}, \qquad \dot{\theta}_2 = \omega_2(\boldsymbol{I}) = \frac{\partial H_N}{\partial I_2}, \tag{7}$$

so that their ratio is no longer constant. We thus find periodic orbit tori (periodic tori for short) densely interspersed among the tori with irrational frequency ratios.

We are now ready to consider the question of time inversion symmetry. This is a property of the $\boldsymbol{q}$-motion for both the original Hamiltonian (1) and the normalized Hamiltonian H_N. There is a known result [20] that the corners of the tori are structurally stable with respect to perturbations that preserve the time-reversal symmetry. The basis for this fact is that self-symmetric non-periodic orbits are dense on the tori on which they lie. The generic caustics of these tori on the $\boldsymbol{P}=0$ plane are hence double folds, whose generic meeting occurs in hyperbolic umbilics, rather than the cusp points of single folds. The addition of symmetric non-harmonic terms to H_N in either the normalized or the original coordinates will not unfold the corners of the tori. It follows that all the tori corresponding to H_N will project as distorted boxes as shown in fig. 1b.

The corners of the boxes lie on the level curve $H_N(0,\boldsymbol{q}) = E$. The $\boldsymbol{q}$-orbits which touch these points have time-reversal symmetry, i.e. they retrace themselves exactly and are referred to as *librations*. A non-periodic torus is densely covered by its librations. This is not the case for periodic tori, with the exception of the degenerate tori, corresponding to a single periodic orbit. Almost all the periodic orbits of the integrable system with the Hamiltonian H_N are therefore pairs of rotations. This statement also holds for each range of periods, since it was obtained individually for each periodic torus, where all periodic orbits have common period determined by the frequencies (7).

The above result does not prevent the librations of an integrable system from being dense. This property indeed follows from the existence of periodic tori arbitrarily close to any quasi-periodic torus. Therefore the dense symmetry orbit in the latter can be arbitrarily well approximated by the very long librations in the former.

For low energies we can account for the small perturbation represented by the remainder of (6) within the framework of the theorem of Kolmogorov, Arnol'd and Moser (KAM, see ref. [19] for example). The result is that most of the tori will only be slightly distorted by the perturbations. Therefore they will still be of the box type. A theorem of Lyapunov [21] and Weinstein [22] also guarantees the survival of both periodic orbits corresponding to infinitely thin periodic tori. Since these touch the energy curve in fig. 1c, they are necessarily librations.

The KAM theorem does not consider the periodic tori. Typically these are broken up, but according to the Poincaré–Birkhoff theorem (see, e.g., ref. [23]) there do remain pairs of isolated stable and unstable periodic orbits. Working directly with (6) so as to obtain *resonant normal forms* as in ref. [19], one finds that usually there only remains a single pair of periodic orbits with the same period as those of the original torus. Many more periodic orbits will appear in the rich *island structure* (see ref. [23] or [10]), but these will have much longer periods.

We will now show that a pair of periodic librations always survives the breakup of a periodic

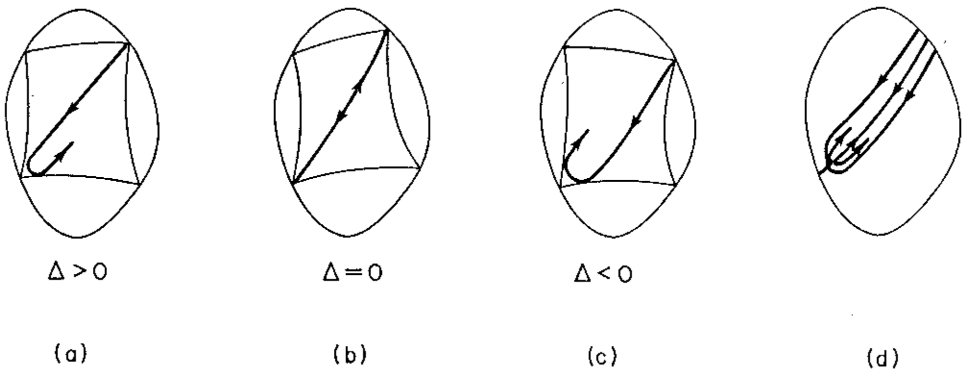


Fig. 2. Tori on the energy shell are specified by a single parameter Δ, such that the libration that starts on the corner is periodic for $\Delta = 0$, as shown in (a), (b) and (c). These librations survive a perturbation that breaks up the periodic torus. The periodic libration still separates the different types of non-periodic librations shown in (d).

box-torus by a perturbation of the normalized Hamiltonian. To this end we first note that each corner of the box corresponds to a single point of an orbit in phase space. Therefore we can follow its superimposed forward and backward $\boldsymbol{q}$-image in time; having finite length, its double image must end in a different corner. There are hence exactly two librations in each unperturbed periodic torus.

Fix now an energy surface and consider the non-periodic tori of H_N in the neighborhood of a given periodic torus and their librations that start out from neighboring corners as in fig. 2. The images of these orbits lie very close to that of the periodic orbit until it reaches its second corner, where there is a parting of ways: the non-periodic librations cannot touch the level curve $H_N(0,\boldsymbol{q}) = E$, lest they should terminate. Assuming that $\mathrm{d}(\omega_1/\omega_2)/\mathrm{d}I_1 \neq 0$ on the periodic torus, then the difference of frequency ratios

$$\Delta = \omega_1/\omega_2 - \alpha, \tag{8}$$

where α is the rational ratio for the periodic torus, changes sign with a change of position of the torus, c.f. the corner of the periodic torus. Therefore, the order in which the orbit touches the two sides of the box near the opposite corner is interchanged when Δ changes sign as shown in figs. 2a, 2b and 2c for $\alpha = 1$.

The version of the KAM theorem for symmetric systems [24] guarantees the existence of tori with irrational frequency ratios close to the rational torus if α is not a low-order rational. There thus exist orbits similar to those of figs. 2a and 2c even in the perturbed system. If we now dismiss the tori and consider the librations as a function of the starting point on the energy level curve, we are faced with a continuous set of curves with the property of being tangent to the level curve in another region, but in two opposite senses, as shown in fig. 2d. The boundary between these two classes must be a periodic libration.

There will be two periodic librations, corresponding to the four corners of the box-torus. There are no more librations, but there may exceptionally be quartets of periodic rotations – symmetric pairs of stable and unstable orbits. Even in this case, the abundance of librations with respect to rotations among short-period periodic orbits will be remarkably enhanced in comparison to that found for the normalized Hamiltonian.

It should be pointed out that general nearly integrable time-reversible systems need not display box-tori of the form we have assumed. For instance, an isotropic system of the form (1) with $V(\boldsymbol{q}) = V(\boldsymbol{q}^2)$ will have symmetric pairs of tori with no corners [20]. Their surviving periodic orbits under general weak perturbation will be rotation pairs rather than librations. However, anharmonic oscillators such as the Hénon–Heiles system form a physically important class of systems that have been the object of an increasing computational literature. Evidently, our results can be immediately generalized to reversible Hamiltonian systems whose integrable tori touch the curve $H(0, \boldsymbol{q}) = E$ in the coordinates presented in the appendix.

3. Bifurcations in time-symmetric systems

The complete classification of the *generic bifurcations* of the periodic orbits in area-preserving maps was obtained by Meyer [15]. This classification applies to almost all the periodic orbits of maps with no special property (such as being the square of another map, for example). Even for maps with some kind of symmetry, however, Meyer's classification holds for periodic orbits that are not constrained in any way by the symmetry. Thus the rotations of a time-symmetric system can be expected to behave generically, since we can impose any change in a rotation as long as this is accompanied by its time-symmetric pair.

The generic classes depend on the ratio $1/n$ of the period of the orbit to that of the *satellite orbits* which coalesce with it at a *periodic n-upling bifurcation*. In all cases there is a single generic form for each period, except for the case with $n = 4$, for which there are two alternative forms. The presence of time-reversal symmetry in the original Hamiltonian system carries over into its Poincaré maps [3]. It was shown by Rimmer [13] that the only effect of this extra symmetry is to add a new possibility for *isochronous bifurcations* ($n = 1$) of symmetric orbits, corresponding to librations of the full system. This new kind of bifurcation will be found with zero probability in general systems or among rotations of time-symmetric systems, but it is likely to occur among librations.

Taking ϵ to be the bifurcation parameter (monotonically related to the energy of the Poincaré section for the full system) the *normal forms* for maps with isochronous bifurcations are given in ref. [17] as

$$S_g(p', q) = qp' + \epsilon q + q^3 + \tfrac{1}{2}p'^2 \tag{9}$$

for the generic bifurcations and, for symmetric bifurcations, the form

$$S_t^{\pm}(p', q) = qp' \pm \epsilon q^2 \pm q^4 + \tfrac{1}{2}p'^2 \tag{10}$$

can be shown to be equivalent to those given by Rimmer [13]. In both cases the central and the satellite periodic orbits are fixed points of the map $(q, p) \to (q', p')$ given implicitly by

$$q' = \frac{\partial S}{\partial p'}, \qquad p = \frac{\partial S}{\partial q}. \tag{11}$$

There exists a canonical transformation that locally takes typical symmetric maps with isochronous bifurcations into one of these normal forms. It is straightforward to see that in the normal coordinates the fixed points for S_g and S_t are, respectively

$$p_g = 0, \qquad q_g = \pm\left(-\tfrac{1}{3}\epsilon\right)^{1/2} \tag{12}$$

and

$$p_t = 0, \qquad q_t = 0, \ \pm\left(-\tfrac{1}{2}\epsilon\right)^{1/2}. \tag{13}$$

Fig. 3 shows the fixed point and invariant curves corresponding to both these typical maps. The $\pm$ sign in eq. (10) corresponds to the two possibilities shown in fig. 3b (the fixed points in eq. (13) are the same for both S^+ and S^-). The generic type (fig. 3a) is known as a *saddle–center bifurcation* and it closely resembles the generic saddle–node bifurcation of dissipative maps (see ref. [25] for example). The orbit structure for the symmetric bifurcation resembles that for the generic period doubling bifurcation ($n = 2$), as does its normal form (10). However, in this case there is a symmetric pair of satellite rotations with the same period, as opposed to a single orbit with double

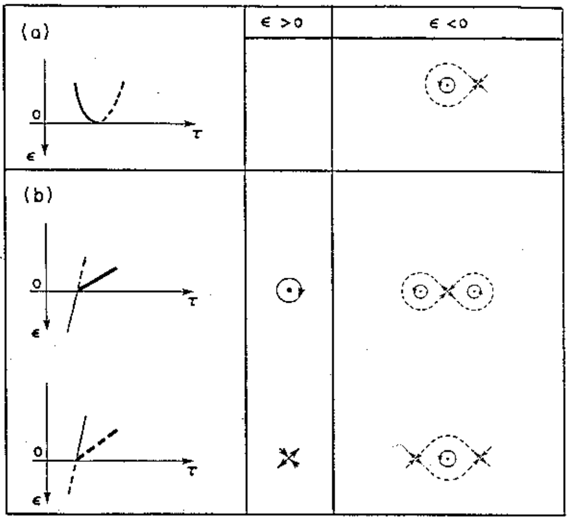


Fig. 3. $\epsilon \times \tau$ plot and invariant curves near the isochronous bifurcation for (a) the generic case and (b) the two symmetric possibilities. In the $\epsilon \times \tau$ plot, stable (unstable) orbits are represented by continuous (dotted) lines. Thicker lines correspond to a symmetry pair of rotations.

the period. The energy-versus-period plot for (12) and (13) is also shown in fig. 3.

What happens to the symmetric bifurcation if we break the time-reversal symmetry? The answer is provided by *catastrophe theory* (see e.g. ref. [16]): The q^3 term in (9) is the germ of the simplest catastrophe – *the fold*. It has *codimension 1*, that is, it can be *unfolded* by the single parameter ϵ (the catastrophic singularity occurs for $\epsilon = 0$). In (10) we also recognize q^4 to be the germ of the next catastrophe – the *cusp*. However, this catastrophe has codimension 2, that is there are two unfolding parameters, whereas there is only ϵ in (10). Thus we can understand (10) to be a special section of the generating function

$$S^{\pm}(p', q) = qp' + \sigma q \pm \epsilon q^2 \pm q^4 + \tfrac{1}{2}p'^2, \tag{14}$$

where the symmetric map is obtained for $\sigma = 0$. The universality of catastrophe-generating functions implies that we can always locally transform the generators of the Poincaré maps for a family of Hamiltonian systems with isochronous bifurcations, so as to coincide with (14). From now on we shall restrict ourselves to $S^+(p', q)$, as the analysis of $S^-(p', q)$ is completely similar.

The map generated by (14) according to (11) is

$$p' = p + \sigma + 2\epsilon q + 4q^3, \qquad q' = q + p, \tag{15}$$

with the fixed points given by

$$p = 0, \qquad 4q^3 + 2\epsilon q + \sigma = 0. \tag{16}$$

The bifurcating periodic orbits also satisfy the supplementary condition that

$$\det|\partial(p', q')/\partial(p, q)| = 0, \tag{17}$$

i.e. in this case

$$12q^2 + 2\epsilon = 0$$

or

$$q = -\left(-\tfrac{1}{6}\epsilon\right)^{1/2} = -\tfrac{1}{2}\sigma^{1/3}. \tag{18}$$

Eliminating the double root $q(\epsilon, \sigma)$ from (16), we thus obtain

$$\epsilon = -\tfrac{3}{2} - \sigma^{2/3} \tag{19}$$

as the cusp-graph shown in fig. 4 for the energy parameter at which the bifurcation occurs as a function of the symmetry-breaking parameter. The single root of (16) is

$$q = \left(-\tfrac{2}{3}\epsilon\right)^{1/2} = -\sigma^{1/3}. \tag{20}$$

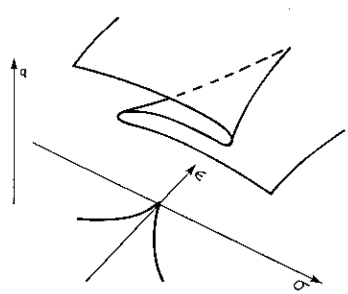
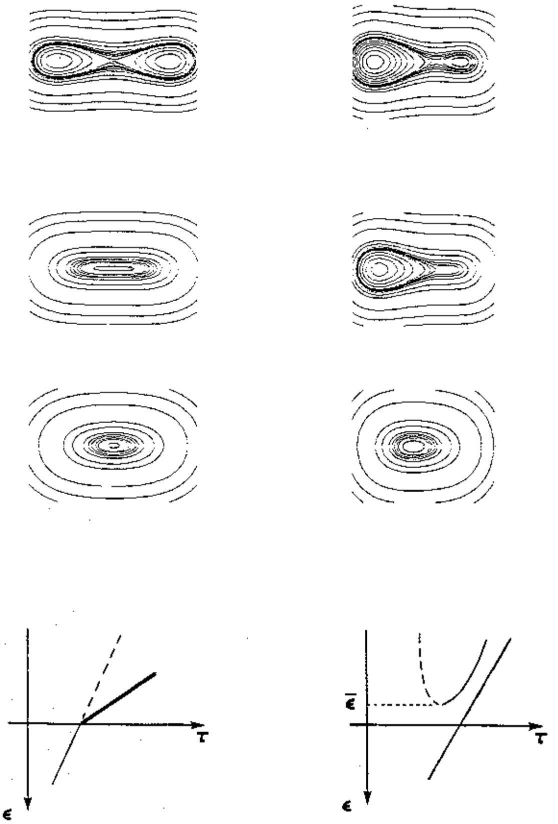
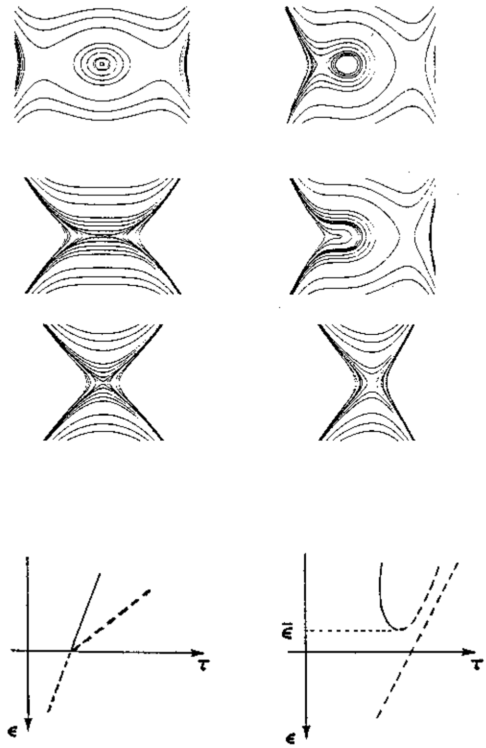


Fig. 4. Fixed points $q = q(\epsilon, \sigma)$ of the map generated by eq. (14). The bifurcations correspond to projection singularities of $q(\epsilon, \sigma)$, specified by the cusp equation $\epsilon = -\frac{3}{2}\sigma^{2/3}$.



(a) (b)

Fig. 5. Invariant curves and $\epsilon \times \tau$ plot for $S^{+}(p, q)$ for (a) $\sigma = 0$ and (b) $\sigma \neq 0$. The notation is the same as for fig. 3.



(a) (b)

Fig. 6. Invariant curves and $\epsilon \times \tau$ plot for $S^{-}(p, q)$ for (a) $\sigma = 0$ and (b) $\sigma \neq 0$. (See fig. 3 for notation.)

For $\sigma \neq 0$ the catastrophe that is obtained by taking ϵ through the value specified by (19) is merely the fold, i.e. we obtain a common saddle–center bifurcation at $p = 0$, $q = (-\frac{1}{6}\epsilon)^{1/2}$. However, the neighboring environment of this bifurcation is not typical due to the presence of another fixed point that does not participate in this bifurcation. This structure is displayed in fig. 5, where a numerical calculation of the invariant curves of the map (15) was performed for both $\sigma = 0$ and $\sigma \neq 0$. Fig. 6 shows the same structure for the map generated by $S^{-}(p', q)$.

So far we have not considered the symmetry of the orbits resulting from a bifurcation. In all the generic bifurcations there either appears a single satellite periodic orbit or a single pair of stable and unstable orbits. It follows that generic bifurcations of librations must result in new librations, because of the absence of symmetric pairs of satellites. Only the symmetric isochronous bifurcation produces a pair of satellites of a new type, that is, a pair of rotations.

Returning to the subject of section 2, we thus find that following a set of librations that exist for low energies of an anharmonic oscillator, there will emerge a large population of new periodic orbits from successive bifurcations. The great majority of these must also be librations. So the prevalence of rotations at long period must have alternative sources in the island structure and homoclinic motion.

4. Effect of bifurcating librations on the energy spectrum

The density of states $n(E)$ for a quantized system with a known classical limit can be formally written as a sum over each mth repetition of all the periodic orbits. Each term has the form

$$\frac{\tau A_m}{2\pi i\hbar}\exp\left(\frac{i}{\hbar}m2\pi J-\tfrac{1}{2}\mu_m\pi\right),\tag{21}$$

where τ is the period for a single repetition,

$$2\pi J=\oint p\,\mathrm{d}\boldsymbol{q}\tag{22}$$

is the action for a single repetition and μ_m is the Maslov index (see e.g. ref. [10]). The form of the amplitude A_m that holds through a bifurcation or *resonance* was found to be [10, 17]

$$A_m=\frac{1}{2\pi i\hbar}\int\mathrm{d}P\,\mathrm{d}Q\left|\frac{\partial^2 S_m}{\partial P\,\mathrm{d}Q}\right|^{1/2}\times\exp\left(\frac{i}{\hbar}\left[S_m(P,Q)-PQ\right]\right).\tag{23}$$

Here (P,Q) are the variables in the Poincaré section and $S_m(P',Q)$ is the generating function for the mth iteration of the Poincaré map.

According to the discussion in section 3, it is only the isochronous bifurcations of librations which may typically differ from those of generic periodic orbits. After a single repetition of the periodic orbits, we thus obtain the amplitude near a bifurcation by merely inserting (9), (10) or (14) in (23). Thus, in the case of a generic bifurcation, integration over P and rescaling $\hbar^{-1/3}Q=x$ leads to

$$A_g=\frac{1}{(2\pi i\hbar^{1/3})^{1/2}}\int\mathrm{d}x\exp\left[i\left(x^3+\epsilon\hbar^{-2/3}x\right)\right].\tag{24}$$

If the two stationary phase points (12) are sufficiently distant, that is

$$(-\epsilon)^{3/2}\gg\hbar,\tag{25}$$

we may treat both stationary points separately, so as to obtain distinct contributions from the stable and the unstable orbits. For both of these the dependence of A_g on Planck's constant is cancelled. If (25) does not hold, however, we must use the full Airy function form of (24) [26]. It is interesting that for small $\epsilon>0$ the bifurcation still contributes to the density of states, though the real periodic orbits no longer exist.

The other case is obtained by substituting (14) into (23), so that integrating over P and identifying $\hbar^{-1/4}Q=x$ we obtain

$$A_t=(2\pi i\hbar^{1/2})^{-1/2}\times\int\mathrm{d}x\exp\left[i\left(x^4+\epsilon\hbar^{-1/2}x^2+\sigma\hbar^{3/4}x\right)\right].\tag{26}$$

The purely symmetric case is specified by $\sigma=0$. The stationary points are then specified by (13), so that the phase difference between these will be large if

$$(-\epsilon)^2\gg\hbar.\tag{27}$$

Therefore, the resonant range of ϵ, where we must treat the orbits collectively, is larger in the semiclassical limit for the symmetric bifurcation than for the generic bifurcation. Also we note that both A_g and A_t diverge right at the bifurcation as $\hbar\to 0$, but A_t has the stronger singularity.

Time-reversal symmetry is broken if $\sigma\neq 0$. The bifurcation is then of the generic type, though in close proximity to a non-participating orbit. Inserting (18) and (20) into (26), we find that the resonance can be separated from the extra orbit only if

$$|\sigma|^{4/3}\gg\hbar.\tag{28}$$

Otherwise, we must use the entire Pearcey function [27] form of (26), even though there is no longer an exact symmetry in the system.

5. Conclusions

Increasing the energy of anharmonic oscillators enhances the remainder of the Hamiltonian with respect to its Birkhoff normal form. The chaotic regions originating in the breakup of the resonant tori will gradually increase and overlap in the manner described by Chirikov in ref. [28]. In this process the low-period orbits surviving the breakup of periodic tori will undergo successive bifurcations, but most of these will not alter the predominance of librations, deduced for the KAM region at low energies. This is in agreement with recent calculations shown in refs. [14, 29, 30]. However, most of these computations were carried out for a system whose potential had a reflection symmetry, so that the Hamiltonian was not generic within the class of those with time-reversal symmetry. Adding further symmetries increases the number of generic bifurcations allowed within the resulting restricted class of Hamiltonians, as shown in refs. [14, 31]. There is therefore much work that can still be done to unravel these more special cases.

We argued in section 1 that as a whole the proportion of librations to rotation pairs must be negligible. Direct evidence of this for chaotic systems is provided by the success of the semiclassical theory for universal statistical properties of the quantum energy spectrum [10–12] that relies exclusively on the pairs of rotations. Even so, these universal properties depend on the limit of long periods. The individual features of the Hamiltonian determine fluctuations in the density of states on a scale that is large in comparison to the level spacing. These are tied to the distribution and amplitude of the short-period orbits. The bifurcations undergone by librations therefore determine a clustering of energy eigenvalues that causes overall peaks in the smooth density of states for anharmonic oscillators [18] at high energies.

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Appendix

A diffeomorphism $\mathbf{R}$ is defined to be a *reversing involution* [3] if it satisfies the two special properties:

(i) $\mathbf{R}^2 =$ identity;

(ii) the dimension of the $\mathbf{R}$-invariant manifold is L if the phase space has dimension $2L$.

The reversibility of the vector field $\dot{x}$ under the corresponding tangent map is expressed by

$$D\mathbf{R}(\dot{x}) = \dot{x}(\mathbf{R}x). \tag{A.1}$$

It is shown by Devaney [3] that the flow ϕ_t generated by a reversible vector field has the property

$$\phi_t = \mathbf{UR}, \tag{A.2}$$

where $\mathbf{U}$ is also a reversing involution. Evidently, the time-reversal symmetry $\mathbf{R}_0$: $(\boldsymbol{p},\boldsymbol{q}) \to (\boldsymbol{p}',\boldsymbol{q}')$ with

$$\boldsymbol{p}' = -\boldsymbol{p}, \qquad \boldsymbol{q}' = \boldsymbol{q} \tag{A.3}$$

is an example of a reversing involution, as is $\phi_t\mathbf{R}_0$, where ϕ_t is the flow for any Hamiltonian with time-reversal symmetry. It is possible to extend the definition of reversibility so as to include non-Hamiltonian systems.

Notice that $\mathbf{R}_0$ defined by (A.3) is *anti-canonical*, that is, its corresponding matrix satisfies the equation

$$\mathbf{R}'\mathbf{J}\mathbf{R} = -\mathbf{J}, \tag{A.4}$$

where

$$\mathbf{J} = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \tag{A.5}$$

and $\mathbf{R}'$ is the transpose of $\mathbf{R}$. Since the flow for a time-reversible Hamiltonian system is canonical, i.e., its Jacobian matrix $\mathbf{M}$ satisfies

$$\mathbf{M}'\mathbf{J}\mathbf{M} = \mathbf{J}, \tag{A.6}$$

we find from (A.2) that all the involutions defined by

$$\mathbf{U} = \mathbf{M}\mathbf{R}_0 \tag{A.7}$$

are also anti-canonical.

Reversible Hamiltonian systems with respect to general anti-canonical involutions comprise a larger class than that of time-reversible systems. It is easy though to construct canonical transformations that reduce the former systems into the latter class. The important point to notice is that the invariant plane for an anti-canonical reserving involution is always *Lagrangian*, i.e. all closed loops on it have zero symplectic area or action. This is because the Jacobian matrix for the flow is $\mathbf{M} = \mathbf{U}\mathbf{R}$ and the invariant surface is defined by $\mathbf{R}x = x$, so on it

$$\mathbf{M}x = \mathbf{U}\mathbf{R}x = \mathbf{U}x. \tag{A.8}$$

It follows that in this surface $\mathbf{M}$ is both canonical and anti-canonical, a contradiction unless the plane is Lagrangian.

We therefore find canonical transformations that will, at least locally, transform the $\mathbf{R}$-invariant surface $p = p_{\mathbf{R}}(q)$ into the $p' = 0$ plane. One example of such transformation taking $\mathbf{R} \to \mathbf{R}_0$ is

$$p' = p - p_{\mathbf{R}}(q), \qquad q' = q \quad (p \geq p_{\mathbf{R}}(q)) \tag{A.9}$$

and

$$x' = -\mathbf{R}_0(\mathbf{R}x) \quad (p < p_{\mathbf{R}}(q)), \tag{A.10}$$

that is

$$p' = -p(\mathbf{R}x), \qquad q' = q(\mathbf{R}x) \quad (p < p_{\mathbf{R}}(q)). \tag{A.11}$$

This transformation is symplectic, because the shear (A.9) is, whereas (A.10) is the product of two anti-symplectic transformations. It is smooth across the invariant surface, since both $\mathbf{R}$ and $\mathbf{R}_0$ are diffeomorphisms.

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