Indices in classical mechanics

Bruno Eckhardt† and Dieter Wintgen‡

† Fachbereich Physik der Philipps-Universität, Renthof 6, W-3550 Marburg, Federal Republic of Germany
‡ Max-Planck Institut für Kernphysik, Postfach 103 980, W-6900 Heidelberg, Federal Republic of Germany

Abstract. We discuss the linearization of the equations of motion around a periodic orbit in a conservative two degree of freedom Hamiltonian system, with an emphasis on computationally useful formulae. Indices are defined using singularities in projections. Conjugate points, self-conjugate points and the possiblity of assigning a symbolic code are discussed.

1. Introduction

Most investigations of nonlinear dynamical systems require the study of periodic motions and their stability properties, e.g. in bifurcation theory. More recently, it has been realized that in strongly chaotic systems periodic orbits form a strictly organized, rigid skeleton, which in turn may be used to evaluate phase space averages; the stability enters in the weights assigned to every orbit (Cvitanović 1988, Artuso *et al* 1990).

However, besides stability, there is another characteristic of trajectories, describing how neighbouring orbits wind around the leading one. This quantity is called the winding number or, because of its relation to singularities, the Morse or Maslov index (by 'index' we mean here any integer assigned to a trajectory). In general dynamical systems, it has attracted attention only recently (e.g. Ruelle 1985, Dressler and Lauterborn 1990) but in semiclassical mechanics this index plays an important and peculiar role (Gutzwiller 1971, Berry and Mount 1972, Eckmann and Sénéor 1976, Percival 1977, Maslov and Fedoriuk 1981). In a previous report (Eckhardt and Wintgen 1990) we have demonstrated that this index can also be used profitably in a purely classical context, namely to assign a symbolic code to trajectories. Numerical experience suggests that this coding is *global*, in contrast to the *local* symbolic codes that follow from the horseshoe construction (Moser 1973). Understanding the global organization of periodic orbits is important for the cycle expansion approach to phase space averages (Cvitanović 1988).

To motivate the connection between the classical coding and the index we recall the basics of pinball scattering (Eckhardt 1987, Gaspard and Rice 1989). Consider an arrangement of convex bodies in the plane and a point particle elastically reflected off the bodies. Once the bodies are labelled, one may code a trajectory by the string of symbols representing the collision sequence. The corresponding quantum problem is to solve the Helmholtz equation $\Delta \psi + k^2 \psi = 0$ for the wavefunction ψ, required to vanish on the surface of the bodies, with appropriate ingoing and outgoing boundary

conditions. Semiclassically, the scattering process is described by the superposition of waves that propagate along classical trajectories with specified ingoing and outgoing momenta, but arbitrary impact parameter. As these waves evolve, their phase increases with the classical action divided by $\hbar$. However, at every collision with the walls of the scattering bodies, there is a phase loss of π due to the boundary conditions. The total accumulated phase loss thus counts the number of collisions with the walls, but it is not directly accessible, since it appears in the exponent and is taken modulo 2π.

What happens classically at these collisions is that a local coordinate system formed of vectors parallel and perpendicular to the trajectory changes orientation. This feature of a collision can easily be carried over to smooth potentials and may be used to define a 'collision with a potential boundary'. If these collisions occur in well separated regions in phase space, one may assign labels to these regions and again code a trajectory by the collision sequence (Eckhardt and Wintgen 1990). Smooth systems differ from billiards in that the change of orientation may take place gradually (a 'rotation' around the orbit) and that the collisions are 'softer', the phase loss being only $\pi/2$.

The above example of a local coordinate system is motivated in position space. The coordinate system corresponds to the projection of 2 out of 4 phase space coordinates into position space. The singularities of this projection both indicate a change of orientation and give rise to the phase loss in semiclassical mechanics. Different local coordinate systems or different projections (say onto position space or onto momentum space or some combination) may yield different positions for singularities, but theorems of differential geometry assure that the total number of singularities is invariant (Milnor 1963, Creagh *et al* 1990). The number of such singularities is a classical index.

In this contribution we discuss some properties of these indices and methods for their calculation. This problem has been considered before by Gutzwiller (1971) for the anisotropic Kepler problem, by Möhring *et al* (1980) for general systems, by Littlejohn and Robbins (1987) for integrable systems and by Creagh *et al* (1990) for unstable orbits. We only consider conservative two degree of freedom Hamiltonian systems, with four-dimensional phase space and three-dimensional energy surface. The equations of motion are given by four first order differential equations, and a 4×4 monodromy matrix relates small deviations from the trajectory at the initial and final point. The stability properties of the trajectory follow from the eigenvalues of this matrix, and the indices we are interested in from its time evolution. The relevant information is contained in a 2×2 submatrix, obtained after elimination of two trivial directions. The elements of the reduced monodromy matrix enter the semiclassical expression for the Green function in position space (Gutzwiller 1971) and the expression for the (Wigner) propagator in phase space (Berry 1989).

The main point of the present paper is to discuss in some detail how the reduced monodromy matrices can be obtained in a computationally useful way and how they relate to other representations, such as those derived from Maupertuis's principle. there is some freedom in the choice of the local coordinate systems; we discuss two, one in 'configuration space' and one in 'phase space'. The labels should not be taken literally (since both systems are of course defined in entire phase space), but more to indicate that they are useful for calculating the entries in the position space Green function and in the phase space Wigner propagator, respectively.

The outline of the paper is as follows. In the next section we discuss the linearized classical motion and introduce the concept of the monodromy matrix. We define two

local coordinate systems and present the reduction of the monodromy matrices and of the linearized equations of motion for them. In section 3, we discuss the winding numbers and their computations. The properties of the different coordinate systems are illustrated for a simple example in section 4. We conclude with some final remarks in section 5.

2. Linearized classical motion

2.1. The monodromy matrix

We will focus on the simplest non-trivial case of a two degree of freedom system with time independent Hamiltonian of the form kinetic plus potential energy,

$$H(\mathcal{Q}, \mathcal{P}) = \mathcal{P}^2/2 + V(\mathcal{Q}) \tag{1}$$

where $\mathcal{Q} = (x, y)$ and $\mathcal{P} = (u, v)$ are coordinates and canonically conjugate momenta, respectively. The equations of motion are

$$\dot{\mathcal{Q}} = \mathcal{P} \tag{2a}$$

$$\dot{\mathcal{P}} = -\partial V/\partial \mathcal{Q} \tag{2b}$$

or,

$$\dot{\gamma} = \mathbf{J}\frac{\partial H}{\partial \gamma} \tag{3}$$

with $\gamma = (\mathcal{Q}, \mathcal{P})$ and $\mathbf{J}$ a 4×4 matrix composed of 2×2 unit matrices $\mathbf{I}$,

$$\mathbf{J} = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix}. \tag{4}$$

A periodic orbit is a periodic solution of the equations of motion (2) or (3), $\gamma_{po}(T) = \gamma_{po}(0)$, where T is the period of the orbit. Since the Hamiltonian is time independent, energy is conserved along the trajectory.

Of central interest here is the behaviour of trajectories in the neighbourhood of periodic orbits. Let a trajectory which starts close to the periodic orbit, $\gamma'(0) = \gamma_{po} + \delta\gamma'$, arrive at the phase space point $\gamma''(T) = \gamma_{po} + \delta\gamma''$ after one period. If the initial displacement is sufficiently small, then the final displacements will be small as well and there is a linear relationship between $\delta\gamma'$ and $\delta\gamma''$,

$$\delta\gamma'' = \mathcal{M}\delta\gamma'. \tag{5}$$

The matrix $\mathcal{M}$ of this linear transformation after a full period is called the monodromy matrix of the periodic orbit. In a slight extension of terminology, we will also refer to $\mathcal{M}(t)$ for intermediate times as monodromy matrix, since a convenient way to find $\mathcal{M}(T)$ is to integrate equations of motion obtained by expanding Hamiltons equations consistently up to first order in the deviations from the orbit. One finds

$$\dot{\mathcal{M}} = \mathcal{L}\mathcal{M} \qquad \mathcal{M}(0) = \mathbf{I} \tag{6a}$$

where the (time-dependent) linearization $\mathcal{L}$ of the flow along the trajectory is given by

$$\mathcal{L} = \mathbf{J}\frac{\partial^2 H}{\partial \gamma^2}\bigg|_{\gamma_{po}(t)}. \tag{6b}$$

The matrix $\mathcal{M}$ is symplectic,

$$\mathcal{M}^+ \mathbf{J} \mathcal{M} = \mathbf{J}. \tag{7}$$

(To see this, differentiate with respect to time and use $\mathcal{L}^+\mathbf{J} - \mathbf{J}\mathcal{L} = 0$). From this property there follow relations between eigenvalues. If λ is a complex eigenvalue, then in general $1/\lambda$, λ^* and $1/\lambda^*$ are eigenvalues as well. As we will show shortly, for a two degree of freedom system two eigenvalues are equal to one, so the remainig two come as a pair λ, $1/\lambda$.

Even without solving the equations of motion for $\mathcal{M}$, we can eliminate two trivial eigendirections. If the initial displacement is along the orbit, then it will be the same after one period. Thus the phase space velocity is an eigenvector to the eigenvalue 1. Similarly, if the displacement leaves the energy shell, then the projection perpendicular to the energy shell is also conserved, since the energies of both trajectories do not change. The non-trivial information in the matrix $\mathcal{M}$ thus concerns the evolution of deviations perpendicular to the orbit on the energy shell. In the next section we will present two coordinate systems that eliminate the trivial directions.

The equations of motion (6) may be derived from a (time dependent) Hamiltonian h,

$$h(\delta\mathcal{Q}, \delta\mathcal{P}) = \tfrac{1}{2}\delta\mathcal{P}^2 + \tfrac{1}{2}\delta\mathcal{Q}^T \mathbf{V}_H \delta\mathcal{Q} \tag{8}$$

where $\mathbf{V}_H = (\partial V/\partial\mathcal{Q}_i\partial\mathcal{Q}_j)$ denotes the Hessian matrix of the potential. We will use only canonical transformations, so the form of the equations and the existence of a Hamiltonian is always assured. However, since the transformations are time dependent, the new Hamiltonian will have additional terms from the derivative of the generator. Using canonical transformations is not strictly necessary (see Gutzwiller 1971) but it shows for instance that the vector normal to the energy shell and the translation along the trajectory are canonically conjugate vectors.

2.2. The monodromy matrix in local coordinates

The monodromy matrix $\mathcal{M}$ consists of the 16 derivatives of final coordinates with respect to initial coordinates, $\mathcal{M}_{ij} = \partial\gamma_i''/\partial\gamma_j'$. An initial displacement along the periodic orbit, $\delta\gamma' = \gamma_\parallel\delta\gamma$ with $\gamma_\parallel = \dot{\gamma}_{po}(0)$, will be mapped back onto itself, $\delta\gamma'' = \delta\gamma'$, whence

$$\gamma_\parallel = \mathcal{M}\gamma_\parallel. \tag{9a}$$

Multiplying equation (9a) with $\mathcal{M}^+\mathbf{J}$ from left and using equation (7) we find $\mathbf{J}\gamma_\parallel$ to be an eigenvector of $\mathcal{M}^+$ with eigenvalue 1,

$$\mathbf{J}\gamma_\parallel = \mathcal{M}^+\mathbf{J}\gamma_\parallel. \tag{9b}$$

By equation (3), the vector $-\mathbf{J}\gamma_\parallel$ is just the gradient of the Hamiltonian and therefore points perpendicular to the energy shell.

To complete our coordinate system, we need two more vectors on the energy shell. We take advantage of the remaining freedom to select coordinate systems satisfying further requirements. One coordinate system is non-singular and well behaved everywhere in phase space. Another is motivated by the desire to obtain the entries in the semiclassical expression for the propagator in configuration space representation. (Here, we will not discuss a related coordinate system that yields the entries for the momentum space representation). To avoid confusion, we will use capital and small letters and indices respectively to distinguish between the two coordinate sets.

2.2.1. Local configuration space coordinates. Our first coordinate system is close to the one introduced by Gutzwiller (1971). We construct the transformation matrix $\mathbf{A}$ from four column vectors, $\mathbf{A} = (\gamma_{\parallel}, \gamma_Q, \gamma_E, \gamma_P)$. The first one is directed along the orbit. The third vector γ_E, points out of the energy shell; we take it to be $\gamma_E = (0, 0, \dot{x}, \dot{y})/p^2$, where $p^2 = \dot{x}^2 + \dot{y}^2$. The normalization is chosen so as to simplify the linearized equations of motion, equation (18) below. The second vector, γ_Q, is a displacement perpendicular to the orbit in configuration space, $\gamma_Q \sim (-\dot{y}, \dot{x}, *, *)$. The non-zero elements marked by stars are necessary to keep the displacement on the energy shell. We take $\gamma_Q = (-\dot{y}, \dot{x}, \alpha\dot{x}, \alpha\dot{y})/p$, where $\alpha = (\dot{x}\dot{v} - \dot{y}\dot{u})/p^2$ follows from the requirement that γ_Q be orthogonal to $\mathbf{J}\gamma_{\parallel}$. The last vector, γ_P, is a displacement of the momenta perpendicular to the orbit in configuration space, $\gamma_P = (0, 0, -\dot{y}, \dot{x})/p$; it obviously remains on the energy shell.

The transformation $\mathbf{A} = (\gamma_{\parallel}, \gamma_Q, \gamma_E, \gamma_P)$ (together with its inverse $\mathbf{A}^{-1}$),

$$\mathbf{A} = \begin{pmatrix} \dot{x} & -\dot{y}/p & 0 & 0 \\ \dot{y} & \dot{x}/p & 0 & 0 \\ \dot{u} & \alpha\dot{x}/p & \dot{x}/p^2 & -\dot{y}/p \\ \dot{v} & \alpha\dot{y}/p & \dot{y}/p^2 & \dot{x}/p \end{pmatrix}$$

$$\mathbf{A}^{-1} = \begin{pmatrix} \dot{x}/p^2 & \dot{y}/p^2 & 0 & 0 \\ -\dot{y}/p & \dot{x}/p & 0 & 0 \\ -\dot{u} & -\dot{v} & \dot{x} & \dot{y} \\ -\alpha\dot{x}/p & -\alpha\dot{y}/p & -\dot{y}/p & \dot{x}/p \end{pmatrix}$$

(10)

is canonical, $\mathbf{A}^+\mathbf{J}\mathbf{A} = \mathbf{J}$, and has determinant one. In these coordinates the monodromy matrix reads

$$\mathbf{A}^{-1}\mathcal{M}\mathbf{A} = \begin{pmatrix} 1 & * & * & * \\ 0 & M_{11} & * & M_{12} \\ 0 & 0 & 1 & 0 \\ 0 & M_{21} & * & M_{22} \end{pmatrix}$$

(11)

where the zeros and ones follow from equations (9) and the normalization of the column vectors in $\mathbf{A}$. The matrix elements marked by a star are in general non-zero but of no further interest. The particular form of the third row expresses energy conservation, whereas the first column is the eigenvector along the periodic orbit. The non-zero matrix elements of the first row are due to the fact that all trajectories are followed for the same time interval T. Their endpoints are not necessarily located in the plane perpendicular to the orbit, even if started there. If the running time of the trajectories are shortened by the amount calculated from the first row, their endpoints will be in that plane.

This coordinate system is peculiar, if the orbit is self-retracing, i.e. runs up to the boundary of the classically allowed region $V(x, y) = E$ where $\dot{x} = \dot{y} = 0$. Then the transformation $\mathbf{A}$ becomes singular: α is well behaved and vanishes at the turning point, but γ_Q and γ_P change their orientation discontinuously, and γ_E diverges. These difficulties can be avoided using orthogonal coordinates in phase space as described in the next section.

The reduced 2×2 matrix $\mathbf{M} = (M_{ij})$ contains the non-trivial information and is called the *Poincaré return map* of the orbit. Its elements M_{ij} are precisely the quantities which enter the semiclassical Green function expressed as the sum over oscillating contributions from classical trajectories (Gutzwiller 1971, Bogomolny 1988). The ampli-

tudes are proportional to $(M_{12}p)^{-1/2}$ and therefore diverge at zeros of M_{12} or at zeros of the speed p. The latter vanishes only at turning points of self-retracing orbits, where usually $M_{12} \neq 0$.

2.2.2. Local phase space coordinates. Alternatively, we may construct a vierbein in phase space using the vector $\gamma_{\parallel}$ pointing along the trajectory, $\gamma_e \sim \partial H/\partial \gamma$ pointing out of the energy shell, and two other vectors constrained only by orthogonality. Normalization of the vectors is again chosen so as to keep the linearization simple. We take

$$\gamma_{\parallel} \qquad \gamma_q = (-\dot{y}, \dot{x}, \dot{v}, -\dot{u})^{\mathrm{T}}/q \qquad \gamma_e = -\mathbf{J}\gamma_{\parallel}/q^2 \qquad \gamma_p = -\mathbf{J}\gamma_q \qquad (12)$$

where $q = |\gamma_{\parallel}|$ is the phase space velocity. As in the preceding section, γ_q and γ_p are perpendicular to the orbit in configuration space, but they differ from γ_Q and γ_P in the elements necessary to ensure orthogonality. Except for trivial cases, the phase space velocity q is always non-zero. Hence the coordinate system is defined everywhere and varies smoothly along the trajectory. The canonical transformation $\mathbf{a}$ and the inverse $\mathbf{a}^{-1}$ read

$$\mathbf{a} = \begin{pmatrix} \dot{x} & -\dot{y}/q & -\dot{u}/q^2 & -\dot{v}/q \\ \dot{y} & \dot{x}/q & -\dot{v}/q^2 & \dot{u}/q \\ \dot{u} & \dot{v}/q & \dot{x}/q^2 & -\dot{y}/q \\ \dot{v} & -\dot{u}/q & \dot{y}/q^2 & \dot{x}/q \end{pmatrix} \qquad \mathbf{a}^{-1} = \begin{pmatrix} \dot{x}/q^2 & \dot{y}/q^2 & \dot{u}/q^2 & \dot{v}/q^2 \\ -\dot{y}/q & \dot{x}/q & \dot{v}/q & -\dot{u}/q \\ -\dot{u} & -\dot{v} & \dot{x} & \dot{y} \\ -\dot{v}/q & \dot{u}/q & -\dot{y}/q & \dot{x}/q \end{pmatrix}. \qquad (13)$$

In these coordinates, the monodromy matrix again takes on the form given in equation (11), but with different non-zero matrix elements. There is a similarity transformation between the non-trivial 2×2 symplectic submatrix $\mathbf{M}$ in the previous coordinate system and $\mathbf{m}$ as obtained from the present one,

$$\mathbf{M} = \begin{pmatrix} 1 & \dot{p}_{\parallel} \\ -\dot{p}_{\parallel} & 1 + \dot{p}_{\perp}^2 \end{pmatrix} \frac{\mathbf{m}}{1 + \dot{p}_{\parallel}^2 + \dot{p}_{\perp}^2} \begin{pmatrix} 1 + \dot{p}_{\perp}^2 & -\dot{p}_{\parallel} \\ \dot{p}_{\parallel} & 1 \end{pmatrix} \qquad (14)$$

where $\dot{p}_{\parallel} = e_{\parallel} \cdot \dot{\mathscr{P}}/p = (\dot{x}\dot{u} + \dot{y}\dot{v})/p^2$ and $\dot{p}_{\perp} = e_{\perp} \cdot \dot{\mathscr{P}}/p = (\dot{x}\dot{v} - \dot{y}\dot{u})/p^2$ are the (normalized) accelerations parallel and perpendicular to the orbit.

The actual matrices $\mathbf{M}$ and $\mathbf{m}$ generally differ in their elements, but contain similar information. For instance, the stability exponent λ, defined as the logarithm of the largest eigenvalue of the monodromy matrix, is the same for both matrices and is given by

$$2\cosh(\lambda) = \mathrm{Tr}(\mathbf{M}) = \mathrm{Tr}(\mathbf{m}). \qquad (15)$$

The winding number may also be obtained from the reduced matrices, but one then needs the equations of motion for $\mathbf{M}(t)$ and $\mathbf{m}(t)$ in local coordinates. These are derived in the next section.

2.3. The linearization in local coordinates

The local coordinate transformations $\mathbf{A}$ and $\mathbf{a}$ separate the non-trivial from the trivial parts of the Hamiltonian flow. We wish to express the linearized equations of motion in these local coordinates, e.g.,

$$\dot{\mathbf{M}} = \mathbf{L}\mathbf{M} \qquad \dot{\mathbf{m}} = l\mathbf{m}. \qquad (16)$$

We find

$$\frac{\mathrm{d}(\mathbf{A}^{-1}\mathscr{M})}{\mathrm{d}t} = \mathbf{A}^{-1}(\mathscr{L}\mathbf{A} - \dot{\mathbf{A}})(\mathbf{A}^{-1}\mathscr{M}) = \mathscr{L}'(\mathbf{A}^{-1}\mathscr{M}) \qquad (17)$$

and an analogous expression for **a**. Evaluation of the matrix products in equation (17) is straightforward but tedious and may be done conveniently with the help of a symbolic manipulation program such as REDUCE. In the configuration space coordinate system (10) equation (17) then yields

$$\mathscr{L}' = \begin{pmatrix} 0 & * & * & 0 \\ 0 & L_{11} & 0 & L_{12} \\ 0 & 0 & 0 & 0 \\ 0 & L_{21} & * & L_{22} \end{pmatrix} \tag{18a}$$

from which the reduced linearization matrix $\mathbf{L} = (L_{ij})$ may be read off,

$$\mathbf{L} = \begin{pmatrix} 0 & 1 \\ -K & 0 \end{pmatrix}. \tag{18b}$$

The zeros in the third row and in the first column of $\mathscr{L}'$ guarantee that the structure (11) of the monodromy matrix is conserved in time. The formal 'curvature' K, is given by

$$\begin{aligned} K &= 3(e_\perp \cdot \dot{\mathscr{P}}/p)^2 + e_\perp^T \mathbf{V}_H e_\perp \\ &= 3\alpha^2 + e_\perp^T \mathbf{V}_H e_\perp \\ &= 3(\dot{x}\dot{v} - \dot{y}\dot{u})^2/p^4 + (V_{xx}\dot{y}^2 + V_{yy}\dot{x}^2 - 2V_{xy}\dot{x}\dot{y})/p^2. \end{aligned} \tag{18c}$$

An equation similar to (18b) may also be derived if the principle of Maupertuis is used (Synge 1926, Whittaker 1961, p 419, Arnold 1978, appendix 1). According to this principle, classical trajectories are geodesics on the 'action surface' with a metric tensor $g_{ij} = 2(E - V)\delta_{ij}$. From this metric one may derive the Riemannian curvature K_R, which then enters into the Jacobi equation for small deviations. However, the curvature K_R,

$$K_R = \frac{(E - V)(V_{xx} + V_{yy}) + V_x^2 + V_y^2}{4(E - V)^3} \tag{19}$$

is *singular* as one approaches the boundary of the classically allowed region! The curvature K (18c), however, is well behaved for self-retracing orbits, even at turning points (as noted before, α vanishes there and the second term approaches a constant).

Comparing the behaviour of the reduced equations (18) and the full transformation (10) near a turning point of a self-retracing orbit, one notes that the local coordinates γ_Q and γ_P change their orientation discontinuously, but the differential equations (18) are smooth. The monodromy matrix **M** is not affected by the abrupt change in the orientation of the coordinate system (see the example in section 4). For orbits passing nearby, however, the orientation of the coordinate system does change and the curvature K in the local equations of motion may become large, causing numerical problems. These 'unnoticed' changes in the orientation of the coordinates at turning points have to be kept in mind when calculating indices (section 3 below).

The calculation for the alternative local coordinate set gives similar results. We find

$$l = \begin{pmatrix} a & b \\ -c & -a \end{pmatrix} \tag{20a}$$

with

$$\begin{aligned} aq^2 &= \dot{x}\dot{u}(V_{yy} - 1) + \dot{y}\dot{v}(V_{xx} - 1) - (\dot{x}\dot{v} + \dot{y}\dot{u})V_{xy} \\ bq^2 &= (\dot{x}^2 + \dot{v}^2)(V_{xx} + 1) + (\dot{y}^2 + \dot{u}^2)(V_{yy} + 1) + 2(\dot{x}\dot{y} - \dot{u}\dot{v})V_{xy} \\ cq^2 &= (\dot{x}^2 + \dot{y}^2)(V_{xx} + V_{yy}) + 2(\dot{u}^2 + \dot{v}^2). \end{aligned} \tag{20b}$$

Now there is no problem with singularities. The behaviour at turning points is smooth since γ_q and γ_p do *not* change their orientation. In fact, the discontinuous turnaround of the configuration space coordinates γ_Q and γ_P is replaced by a smooth rotation of the phase space coordinates. This will be illustrated in section 4 for a simple example.

Finally we note that the local coordinate systems defined by equations (10) and (12) are identical whenever the acceleration $\ddot{\mathscr{P}}$ vanishes, e.g. in a local extremum of the potential. For billiard systems this is globally fulfilled. The final monodromy matrices $M(T)$ and $m(T)$ after one period are then identical, see equation (14), but their derivatives generally differ! The reason for this is that even though the transformations A and a are identical, $\dot{A}$ and $\dot{a}$ and hence L and l are different.

2.4. Discrete symmetries: the monodromy matrix in the fundamental domain

Rather often, dynamical systems have discrete symmetries such as reflections on planes or rotations in configuration space. It is then convenient to desymmetrize the problem by going into the fundamental domain (Cvitanović and Eckhardt 1989). All information of the full motion is contained in the desymmetrized motion of the fundamental domain.

The discrete symmetry can also show up in that the trajectory passes through a symmetry image of the initial condition after some fraction of the period. The further evolution may then be obtained from symmetry images of the initial segment. The action of the orbit and the period, being scalars, are simply additive under the symmetry transformations. The monodromy matrix, however, is sensitive to the type of symmetry transformation.

Specifically, let us consider a potential V with reflection symmetry around the y-axis, $V(x, y) = V(-x, y)$. A symmetric periodic orbit of period T starting from $\gamma_{po}(0)$ will have reached $\gamma_{po}(T/2) = \Pi_x \gamma_{po}(0)$ after time $T/2$, where

$$\Pi_x = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{21}$$

It will therefore appear closed with the period $T/2$ in the fundamental domain, where γ_{po} and $\Pi_x \gamma_{po}$ are identified. for the linearization this means that we can write

$$\mathscr{M}(T) = (\Pi_x \mathscr{M}(T/2))^2. \tag{22}$$

The reduced monodromy matrix M in the fundamental domain may be read off from $A^{-1}(0)\Pi_x\mathscr{M}(T/2)A(0)$. As a result, all element of M change sign. In particular, the type of an unstable periodic orbit changes from hyperbolic to inverse hyperbolic and vice versa.

The sign change occurs for reflections only; for rotations the matrix elements remain the same.

3. The winding number and classical indices

The monodromy matrices are not invariant under linear transformations but their eigenvalues (or equivalently the trace and the determinant) are. For stable periodic orbits the eigenvalues may be written in the form $e^{\pm 2\pi i \phi}$ where ϕ is the winding number. It describes the number of turns of neighbouring trajectories around the reference

orbit in phase space. For unstable orbits, the eigenvalues are real pairs, either $e^{\pm\lambda}$ (hyperbolic orbit) or $-e^{\pm\lambda}$ (inverse hyperbolic orbit) with λ the stability exponent (the Lyapunov exponent Λ is a divergence rate, $\Lambda = \lambda/T$). Nevertheless, by following the monodromy matrix along the orbit, one can define a winding number. Formally, the eigenvalues are then $\exp \pm(\lambda + 2\pi i\phi)$ where ϕ can take on integer (hyperbolic orbit) or half integer (inverse hyperbolic orbit) values only. Hence, for unstable orbits the discrete value 2ϕ can be viewed as a classical index.

In the next section we will describe how to compute the winding number ϕ for unstable orbits. For stable orbits only minor additional considerations are necessary, which are described at the end of the chapter.

3.1. The winding number in global coordinates

The polar decomposition theorem for symplectic matrices says that any such matrix may be written uniquely as a product of two symplectic matrices, one positive definite symmetric (**T**) and one orthogonal (**R**) (Littlejohn 1986). Writing $\mathcal{M}$ in the form of block 2×2 matrices (coordinates being as previously $\mathcal{Q}, \mathcal{P}$), one finds

$$\mathcal{M} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} = \begin{pmatrix} \mathbf{T}_1 & \mathbf{T}_2 \\ \mathbf{T}_2^+ & \mathbf{T}_3 \end{pmatrix} \begin{pmatrix} \mathbf{R}_1 & \mathbf{R}_2 \\ -\mathbf{R}_2 & \mathbf{R}_1 \end{pmatrix}. \tag{23}$$

The winding number is contained in the orthogonal transformation **R**, since $\det(\mathbf{R}_1 + i\mathbf{R}_2) = \exp(2\pi i\phi)$ is just a phase. In practice, it is not necessary to decompose $\mathcal{M}$, because the determinant of $\mathbf{A} + i\mathbf{B}$ can also be used to determine ϕ. To see this, calculate

$$\det(\mathbf{A} + i\mathbf{B}) = e^{2\pi i\phi} \det(\mathbf{T}_1) \det(\mathbf{I} + i\mathbf{T}_1^{-1}\mathbf{T}_2). \tag{24}$$

From the definition of **T** it follows that $\mathbf{T}_1$ is positive definite and $\mathbf{T}_1^{-1}\mathbf{T}_2$ is real symmetric. Hence the total phase ψ of the determinant equals

$$\psi = \arg\det(\mathbf{A} + i\mathbf{B}) = 2\pi(\phi + \nu). \tag{25}$$

The contribution ν of the complex determinant on the RHS of equation (24) is bounded between 0 and $\frac{1}{2}$. Furthermore, ψ increases monotonically in time because $\dot{\psi}$ is positive definite for Hamiltonians of the form (1) (Littlejohn 1988). Hence ϕ is determined uniquely from $\det(\mathbf{A} + i\mathbf{B})$: During the period T the imaginary part of $\det(\mathbf{A} + i\mathbf{B})$ changes sign exactly n times, with n given by $n = 2\phi$.

3.2. The winding number in local coordinates

The determination of the winding number in local coordinates is quite similar. For the configuration space coordinates (10) the analogue of the imaginary part of the determinant (25) is just the matrix element M_{12}. Again, the phase $\psi = \arg(M_{11} + iM_{12})$ is monotonically increasing since $\dot{\psi} > 0$. Whenever $M_{12}(t)$ equals zero we have a *conjugate point*, which is a focus for neighbouring trajectories. At a *self-focal point*, $M_{12}(T) = 0$; then trajectories started on the periodic orbit in configuration space but with different momenta all return to the starting point. That is to say, deviations in momentum space are mapped within momentum space. This also means that either the stable or unstable manifold points in momentum direction. In this sense, selffocal points are caustics of the stable and unstable manifolds. There are twice as many selffocal points as caustics on a manifold, and the number of caustics is just twice the winding number 2ϕ (Creagh *et al* 1990).

Self-focal points divide the trajectory into segments with different numbers of conjugate points. The number of conjugate points equals the maximal one, if the sign of $M_{12}(T)$ equals the sign of the trace of $\mathbf{M}(T)$; otherwise there is one less. The maximal number of conjugate points equals half the number of self-focal points. The index 2ϕ is given by the maximal number of conjugate points. However, we have to add an additional index whenever $\mathcal{P} = 0$, e.g. when the trajectory passes a turning point of a self-retracing orbit: the local coordinates change their orientation discontinuously, but the monodromy matrix $\mathbf{M}$ remains regular by 'ignoring' this change. Topologically, this type of index belongs to a cusp in the invariant manifolds.

For the phase space coordinates (12) things change slightly. First of all there is no simple geometrical interpretation for the *self-conjugate* points, where $m_{12}(T) = \partial\gamma_q''/\partial\gamma_p'$ vanishes. The reason is that in contrast to γ_P the phase space vector γ_p also contains a displacement in the positions. Nevertheless, γ_p is still directed along a stable (or unstable) invariant manifold, but the self-conjugate point is not related to a focus in coordinate space (for this reason we call them self-conjugate instead of self-focal points). The second difference is that generally the phase ψ of $m_{11} + im_{12}$ does not increase monotonically. We find $\text{sign}(\dot\psi) = \text{sign}(b)$, where b is the l_{12}-element of the linearization matrix (20). Nevertheless, the bookkeeping for computing the winding number is simple. We have to determine the maximal number of conjugate points as described above, but each conjugate point (including the starting point) is now weighted with the sign of b. There is no extra index for turning points, because the transformation $\mathbf{a}$ is non-singular.

3.3. The winding number of stable orbits

For stable orbits the eigenvalues of the reduced monodromy matrices equal $e^{\pm iu} = e^{\pm 2\pi i\phi}$, but from the logarithmic eigenvalue $|u|$ alone it is not possible to determine ϕ. The computation of ϕ is simpler in local coordinates, where it is possible to determine ϕ uniquely after one period. In global coordinates multiple traversals of the periodic orbit must also be considered because of the additional phase ν appearing in the total phase ψ of the determinant (25). Hence, we have to test whether

$$\phi = \begin{cases} n/2 + |u|/2\pi & n \text{ is even} \\ (n+1)/2 - |u|/2\pi & n \text{ is odd} \end{cases} \tag{26}$$

is compatible with mutiple traversals j of the oribt, where ϕ_j must equal $j\phi$. In (26), n is defined as the integer part of the total phase ψ divided by π, i.e. as the number of changes of sign of the imaginary part of $\det(\mathbf{A} + i\mathbf{B})$. If the hypothesis (26) is incompatible with the results for multiple traversals, ϕ is given by (26) with n replaced by $n-1$.

It is much easier to determine the winding number using the local phase space coordinates (12). Since there are no self-conjugate points for stable orbits, the number n of conjugate points (including the weights) *always* equals the integer part of 2ϕ. Hence ϕ is determined by equation (26) already after one period. Calculating ϕ using the local configuration space coordinates (10) is only slightly more involved: we have to add $\frac{1}{2}$ for each turning point along the orbit.

Finally we note, that the analysis presented in this chapter is independent of whether we study the monodromy matrix of the full domain or the matrix of the desymmetrized fundamental domain. Of course, one has to count only changes of sign in the continuous flow of the appropriate matrix elements, not those induced by discrete transformations

to obtain the monodromy matrix in the fundamental domain. It follows then, that the relation between the type of hyperbolic fixed points and the winding number generally *is lost*: It is only for the motion in the full domain that a periodic orbit is (inverse) hyperbolic when the winding number is (half) integer.

4. An example

Consider the Hamiltonian

$$H(\mathcal{Q}, \mathcal{P}) = u^2/2 + v^2/2 + x^2/2 - \Lambda^2 y^2/2. \tag{27}$$

It has an unstable periodic orbit running along the x-axis,

$$
\begin{aligned}
x(t) &= x_0 \cos(t) + u_0 \sin(t) & y(t) &= 0 \\
u(t) &= -x_0 \sin(t) + u_0 \cos(t) & v(t) &= 0.
\end{aligned}
\tag{28}
$$

A trajectory started on the orbit with a little momentum in the y-direction does not return, so one would not expect to find self-focal points. After one period the monodromy matrix $\mathcal{M}$ in cartesian coordinates is given by

$$
\mathcal{M} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \cosh(\Lambda T) & 0 & \sinh(\Lambda T)/\Lambda \\
0 & 0 & 1 & 0 \\
0 & \Lambda \sinh(\Lambda T) & 0 & \cosh(\Lambda T)
\end{pmatrix}.
\tag{29}
$$

The matrix $\mathcal{M}$ already has the desired form (11), because the local coordinates γ_Q and γ_P accidently coincide with the global coordinates y, v (the orientation may differ however). Thus the transformation to configuration space coordinates does not alter $\mathcal{M}$. The matrix element $M_{12} = \sinh(\Lambda T)/\Lambda$ is indeed always non-zero, so there are no self-focal points. Even though the transformation **A** does not alter the form of the monodromy matrix after one period, the relations between local and global coordinates do change along the orbit, even for the coordinates perpendicular to the orbit. The transformation **A** has the form

$$
\mathbf{A} = \begin{pmatrix}
u & 0 & 0 & 0 \\
0 & \text{sign } u & 0 & 0 \\
-x & 0 & 1/u & 0 \\
0 & 0 & 0 & \text{sign } u
\end{pmatrix}.
\tag{30}
$$

The discontinuity of γ_Q (second column vector) and γ_P (fourth vector) and the divergence of γ_E (third vector) at the turning point $u = 0$ is obvious. Nevertheless, the differential equation (16) for the linearized motion in the configuration space coordinates remains regular. The curvature K, (18c), is constant and simply given by $K = -\Lambda^2$.

In the phase space coordinates (12), the linear transformation matrix is

$$
\mathbf{a} = \begin{pmatrix}
u & 0 & x/q^2 & 0 \\
0 & u/q & 0 & -x/q \\
-x & 0 & u/q^2 & 0 \\
0 & x/q & 0 & u/q
\end{pmatrix}.
\tag{31}
$$

This matrix is nowhere singular, since the phase space velocity $q^2 = u^2 + x^2 = 2E_0$ never vanishes. Of the transformed matrix $\mathbf{a}^{-1}\mathcal{M}\mathbf{a}$ we only list the interesting submatrix $\mathbf{m}$,

$$\mathbf{m} = \begin{pmatrix} \cosh(\Lambda T) + \dfrac{ux(\Lambda^2+1)}{\Lambda q^2}\sinh(\Lambda T) & \dfrac{u^2 - \Lambda^2 x^2}{\Lambda q^2}\sinh(\Lambda T) \\ \dfrac{\Lambda^2 u^2 - x^2}{\Lambda q^2}\sinh(\Lambda T) & \cosh(\Lambda T) - \dfrac{ux(\Lambda^2+1)}{\Lambda q^2}\sinh(\Lambda T) \end{pmatrix}. \tag{32}$$

In this coordinate system the periodic orbit has self-conjugate points, since $\mathbf{m}$ can have vanishing off-diagonal elements; the upper right corner vanishes whenever $u^2 = \Lambda^2 x^2$ and the lower left corner element vanishes for $x^2 = \Lambda^2 u^2$.

The calculation of the classical index is simple in both coordinate systems. In the phase space coordinates there are four self-conjugate points along the periodic orbit, hence $\phi = 1$. Using configuration space coordinates we arrive at the same result: there is no self-focal point, but two turning points. This supports our statement that in the configuration space coordinate system the winding number is the number of zeros of $M_{12}(t)$ plus the number of the reversals, whereas in the phase space coordinate system, only the zeros of $m_{12}(t)$ need to be counted.

The transformation to phase space coordinates regularizes the discontinuities of the configuration space coordinates at turning points by a smooth rotation of the coordinates perpendicualar to the orbit. This is why indices coming from turning points appear as indices from additional conjugate points in the phase space representation. This smooth rotation is obvious in the present example: In both coordinate systems, the non-trivial coordinates only have components in (y, v) direction. The transformations $\mathbf{A}_\perp$ and $\mathbf{a}_\perp$ relating global (y, v) coordinates to the local ones $((\gamma_Q, \gamma_P)$ and (γ_q, γ_p), respectively) are

$$\mathbf{A}_\perp = \begin{pmatrix} \text{sign } u & 0 \\ 0 & \text{sign } u \end{pmatrix} \qquad \mathbf{a}_\perp = \begin{pmatrix} u/q & -x/q \\ x/\dot{q} & u/q \end{pmatrix}. \tag{33}$$

Since $\mathbf{A}_\perp$ and $\mathbf{a}_\perp$ are symplectic orthogonal, they coincide with the orthogonal matrix $\mathbf{R}$ in the polar decomposition. For the configuration space coordinates, the phase $\arg \det(R_{11} + iR_{12})$ jumps discontinuously by π at the turning points, but in the phase space coordinates, it increases smoothly by 2π.

This type of regularization is a general feature of the transformation from configuration space to phase space coordinates and is not restricted to the simple example given above. To see this, we calculate the polar decomposition $\mathbf{TR}$ of the matrix connecting $\mathbf{M}$ and $\mathbf{m}$, equation (14). We find $\arg \det(R_{11} + iR_{12}) = e^{i\beta}$ with $\tan \beta = 2\dot{p}_\parallel/(2 + \dot{p}_\perp^2)$. If there is no turning point along the trajectory $\dot{p}_\parallel$ will always be finite; hence $\beta(T) = \beta(0)$ and the winding number associated with this transformation is zero. However, if the orbit is self-retracing, $\dot{p}_\parallel$ will diverge at the (two) turning points and $\beta(T)$ increases by 2π. The singularity at each turning point in the configuration space representation gives rise to two additional self-conjugate points (one for each invariant manifold) in the regularized phase space representation.

5. Concluding remark

The transformation to the local position space coordinate system (10) is very useful for the standard approach to the semiclassical Green function, whereas the phase space

coordinates (12) are more appropriate for calculating the semiclassical Wigner propagator. After one period, equation (14) yields the transformation between both monodromy matrices. For the semiclassical density density of states only the winding number and the trace of the monodromy matrix are needed.

The main advantage of the phase space coordinate system is that it is non-singular everywhere and that the corresponding linearized equations of motion (20) are numerically well behaved. The configuration space coordinate system has discontinuities for self-retracing orbits. Even though the linearized equations of motion are non-singular, they can be cumbersome in numerical applications. The equations of motion derived from the principle of Maupertuis are numerically useless because they are singular at the boundary points. In this sense, we have achieved a regularization of Jacobi's equation of motion for small deviations from a periodic trajectory (Synge 1926).

As to the assignment of symbols to periodic orbits, they require the identification of 'collision' regions in phase space, and these may be easier to locate in one coordinate system than in another (Eckhardt and Wintgen 1990). Nevertheless, certain properties of the orbit, such as its symbol length, are invariant if defined via the classical index.

We therefore expect that even if there is no immediate interpretation of the index in terms of collisions, as e.g. in the anisotropic Kepler problem (Gutzwiller 1973, 1977) or the collinear helium atom (Ezra *et al* 1991), the index will be a useful guide in the search for a symbolic code.

Extensions of the calculations presented here to more than two degrees of freedom are conceivable, but presumably analytically rather involved. The dimension of the reduced matrices **M** then becomes $2(n-1) \times 2(n-1)$ for n degrees of freedom and the index can be based on degeneracies (vanishing determinants) of $(n-1) \times (n-1)$ submatrices. If the regions in phase space where these singularities occur are sufficiently separated, then one may label them and code trajectories by their visitation sequence. Complications can be expected from the possiblity that at the singularity the rank of these submatrices may be reduced by two or more rather than just one. An obvious pinball analogue is a point particle scattered elastically off several spheres in three-dimensional space (Chen *et al* 1990).

Acknowledgments

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