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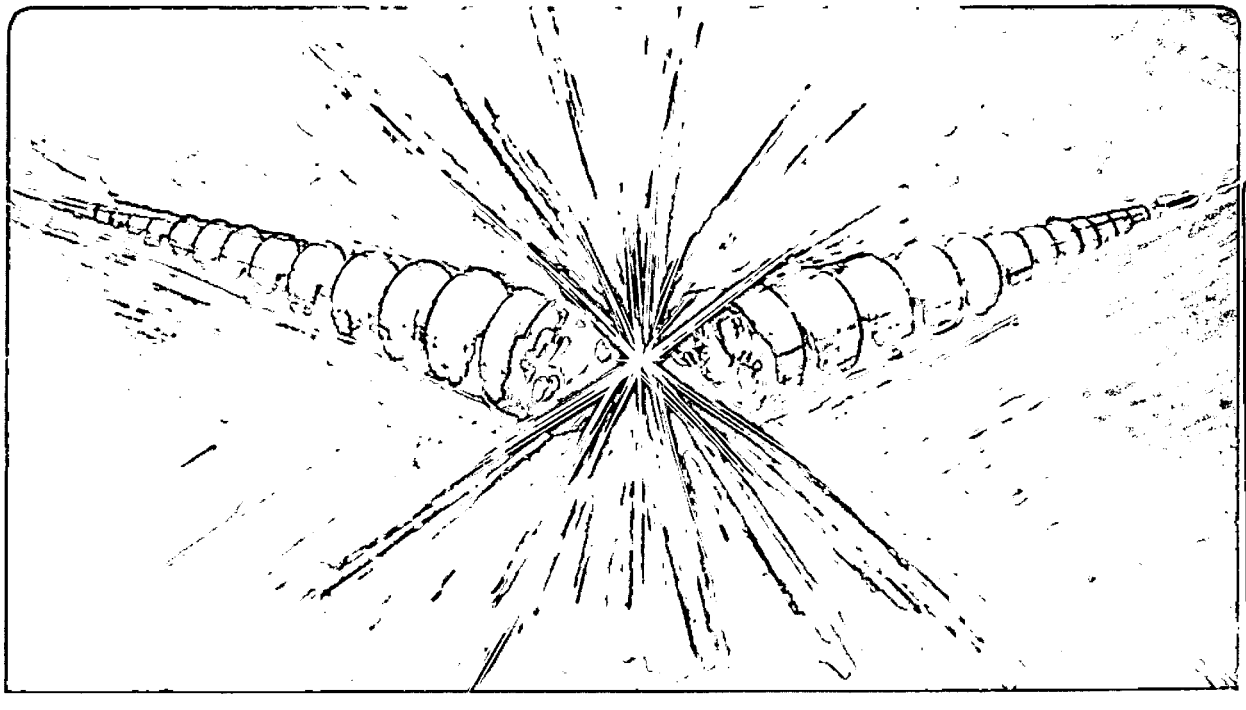

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Geometrical Properties of Maslov Indices in the Semiclassical Trace Formula for the Density of States

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Abstract

We show that in the trace formula of Gutzwiller and Balian and Bloch, applied to systems of two degrees of freedom, the Maslov index arising in the contribution from each periodic orbit is equal to twice the number of times the stable and unstable manifolds wind around the periodic orbit. As a consequence, we find that the Maslov index of a periodic orbit is equal to the Maslov index defined by either its stable or its unstable manifold. In this way it becomes apparent that the Maslov index occuring in the trace formula is an intrinsic property of the periodic orbit, being independent of the coordinates used to find it. In contrast to the case of torus quantisation applied to integrable systems, where only even Maslov indices appear, we find that odd Maslov indices can arise in the trace formula of chaotic systems. These odd Maslov indices arise in the contributions of periodic orbits that are hyperbolic with reflection.

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1. Introduction

In this paper we will examine the geometrical properties of the Maslov index appearing in the trace formula of Gutzwiller[1] and Balian and Bloch,[2]

$$\rho(E) \approx \frac{1}{\pi\hbar} \sum_{\text{po's}} \frac{T}{|\det(M-I)|^{\frac{1}{2}}} \cos\left(\frac{1}{\hbar}S - \sigma\frac{\pi}{2}\right). \tag{1.1}$$

Here the density of states $\rho(E)$ of a quantum mechanical system is expressed approximately as a sum over the periodic orbits of the corresponding classical system. In this formula M is the stability matrix of the orbit, T is the period of the primitive orbit and σ is the Maslov index of the orbit.

An examination of the derivation of Eq. (1.1) reveals that σ is a sum of two contributions. The first is the Maslov index of the energy-dependent Green's function, which can be derived from a count of caustics along the periodic orbit. The second contribution arises when one takes the trace of the energy-dependent Green's function to get the sum over periodic orbits; this contribution is determined by the stability matrix M. While correct, the determination of σ from this relationship is somewhat unsatisfactory because the method is not manifestly phase space invariant. Each of the contributions to σ depends on the phase space coordinates being used. On the other hand, the other quantities appearing in Eq. (1.1), T, $\det(M-I)$ and S, are obviously independent of the canonical coordinates used to compute them; we should expect the same to be true for σ. It is this problem that motivates us to seek a coordinate-free, geometrical interpretation for σ.

We will show that, for systems of two degrees of freedom, σ is equal to twice the number of times the stable and unstable manifolds wind around the periodic orbit over a single traversal of it. We determine the number of windings by following the stable and unstable manifolds (which we will often refer to, collectively, as the invariant manifolds) as they evolve in surfaces of section that are constructed along the length of the orbit. With this interpretation our goal of finding an intrinsic determination of σ is achieved; the winding number is independent of the coordinate system used.

In fact we can go one step further and remove reference even to the surfaces of section. It turns out that periodic orbits have associated to them, in a canoni-

cally invariant way, a winding number.[3] This follows from the observation that the invariant manifolds of periodic orbits are Lagrangian, so that periodic orbits may be regarded as closed curves on Lagrangian manifolds. According to a theorem of Arnol'd,[5] the Maslov index of such a curve is given by a winding number, and as such is a canonical and topological invariant. It is natural to conjecture that, in any number of dimensions the index σ in the trace formula is just this winding number.[4] With our calculations we can prove this in the two-dimensional case. In this way the Maslov index is placed on the same footing as say, the the Maslov indices of invariant tori, μ_j, that appear in the torus quantisation condition $I_j = (n_j + \mu_j/4)\hbar$. We would like to stress that, until now, it has not been shown that the index occurring in the trace formula is a Maslov index in the usual sense.

A central idea of this paper, due to one of us (JMR), is that periodic orbits have winding numbers, and that these are related to Maslov indices. Since the completion of the work described in this paper, considerably deeper insight into this relationship has been obtained and will be reported on in the future.[3]

The paper is organised as follows. In Sec. (2) we review some of the basics that are needed for the derivation of the trace formula. We state the WKB approximation for the energy-dependent Green's function and review multidimensional WKB theory in preparation for finding the Maslov index of the Green's function. In Sec. (3) we examine the Maslov index of the energy-dependent Greens function within the context of multidimensional WKB theory. We show how it can be determined from a reduction of the dynamics to surfaces of section that are constructed along the classical trajectories contributing to the Green's function. In Sec. (4) we examine what happens when one computes the trace of the energy-dependent Green's function. Following the original derivation of Gutzwiller[1] we find that extra contributions to the index arise, over and above the Maslov index of the energy-dependent Green's function. In Sec. (5) we interpret the contributions to σ geometrically in the surfaces of section and find that σ is twice the winding number of the invariant manifolds in the surfaces of section. Finally, in Sec. (6) we explore some of the geometrical aspects of σ that make use of the full phase space and are independent of the surfaces of section.

2. Background material

In this section we review some of the elementary facts that we will use later on. In 2.1 we write down the WKB formula for the energy-dependent Green's function and indicate how the trace formula is obtained from it. In 3.2 we state the rules for determining Maslov indices in multidimensional WKB theory.

2.1 Foundations for periodic orbit theory.

The trace formula Eq (1.1) is based on the following identity relating the density of states $\rho(E)$ of some Hamiltonian H to the trace of its energy dependent Green's function, $G(\mathbf{x},\mathbf{x}',E)$:

$$\rho(E) = -\frac{1}{\pi}\,\mathrm{Im}\int d\mathbf{x}\, G(\mathbf{x},\mathbf{x},E). \tag{2.1.1}$$

The energy dependent Green's function is defined by

$$G(\mathbf{x},\mathbf{x}',E) \equiv \langle \mathbf{x}|\frac{1}{E-H}|\mathbf{x}'\rangle. \tag{2.1.2}$$

The basic idea is to use the following semiclassical approximation for $G(\mathbf{x},\mathbf{x}',E)$ as a sum over classical paths:

$$G(\mathbf{x},\mathbf{x}',E) \approx \frac{1}{i\hbar}\frac{1}{(2\pi i\hbar)^{(N-1)/2}}\sum D(\mathbf{x},\mathbf{x}',E)e^{\frac{i}{\hbar}S(\mathbf{x},\mathbf{x}',E)-i\mu\pi/2}, \tag{2.1.3}$$

where the sum is taken over all the classical trajectories that go from $\mathbf{x}'$ to $\mathbf{x}$ at energy E. N is the number of degrees of freedom, the phase $S(\mathbf{x},\mathbf{x}',E)$ is the action of the trajectory,

$$S(\mathbf{x},\mathbf{x}',E) = \int_{\mathbf{x}'}^{\mathbf{x}} \mathbf{p}\cdot d\mathbf{x}, \tag{2.1.4}$$

the amplitude $D(\mathbf{x},\mathbf{x}',E)$ is the following $(N+1)\times(N+1)$ determinant,

$$D(\mathbf{x},\mathbf{x}',E) = \begin{vmatrix} \frac{\partial^2 S}{\partial\mathbf{x}\partial\mathbf{x}'} & \frac{\partial^2 S}{\partial\mathbf{x}\partial E} \\ \frac{\partial^2 S}{\partial\mathbf{x}'\partial E} & \frac{\partial^2 S}{\partial E\partial E} \end{vmatrix}^{\frac{1}{2}}, \tag{2.1.5}$$

and μ is the Maslov index. Note that each of S, D and μ depends on the path. In this paper, we will be particularly interested in μ

The trace formula Eq. (1.1) is obtained by evaluating the integral in Eq.(2.1.1) by the stationary phase approximation. In doing so one finds contributions only from particular paths, the periodic orbits, and the result is the sum over periodic orbits in Eq. (1.1)

We will not discuss in detail the derivation of Eq. (2.1.3). We just point out that the usual derivations begin with the propagator, or time-dependent Green's function $K(\mathbf{x},\mathbf{x}',t)$, for which an approximation similar to Eq. (2.1.3) can be derived from the path integral or from WKB theory. This approximation for $K(\mathbf{x},\mathbf{x}',t)$ is a sum over classical paths like the one in Eq. (2.1.3), except that the sum is taken over trajectories of a given time rather than energy. The energy-dependent Green's function is related to the propagator by a Laplace transform in time, which can be evaluated by the stationary phase approximation. Doing so yields the sum over trajectories of a given energy that we see in Eq. (2.1.3).

When the classical dynamics is chaotic (as is the case for the systems we want to consider) the exponential separation of orbits makes the semiclassical approximations break down after times of order $|\ln\hbar|$. In particular the WKB propagator $K(\mathbf{x},\mathbf{x}',t)$ is not valid for times $t > O(|\ln\hbar|)$. On the other hand, in deriving Eq. (2.1.3) one needs to use the WKB propagator for arbitrarily long times. One can overcome this problem by giving E a positive imaginary part $i\epsilon$. This has the effect of introducing an exponential cutoff in time, $e^{-\epsilon t/\hbar}$, in the Laplace transform that relates $G(\mathbf{x},\mathbf{x}',E)$ to $K(\mathbf{x},\mathbf{x}',t)$, thus removing the effect of long-time orbits.

Treating the classical dynamics for complex E is fraught with difficulties however and is not something we wish to deal with in this paper. In order to overcome the difficulties with long-time orbits we will take the point of view that Eq. (2.1.3) should include only orbits that take less than some cutoff time $t_c \sim O(|\ln\hbar|)$. In addition to errors of higher order in $\hbar$ therefore, Eq. (2.1.3) will contain errors due to the neglect of the long-term dynamics. The effect on the trace formula is that $\rho(E)$ is only determined to within a finite resolution $\Delta E \sim \hbar/t_c \sim O(\hbar/|\ln\hbar|)$. More precisely, fluctuations in $\rho(E)$ on energy scales ΔE or larger will be faith-

fully reproduced by the trace formula but fluctuations on finer energy scales will be averaged over.

With these problems in mind we will proceed with the main purpose of this paper, which is an examination of the Maslov index. Finding the Maslov index in Eq. (2.1.3) by tracing through the derivation outlined above is rather complicated. We must first find the Maslov index for the propagator. Having done this, we find the index occurring in the energy-dependent Green's function by taking into account extra phase contributions that arise in performing the Laplace transform by the stationary phase approximation. Writing the Maslov index of the energy-dependent Green's function in terms of the the Maslov index of the propagator like this is unnecessarily complicated. While everything else in Eq. (2.1.3) is determined completely by the classical trajectories of a fixed energy this approach forces us to consider other trajectories in order to find the Maslov index. This seems somewhat unnatural. It would much easier if we could determine the Maslov index in the energy-dependent Green's function directly, without reference to the propagator.

We can do this if we realise that Eq. (2.1.3) is a special case of general multidimensional WKB approximations for wavefunctions. Within this theory the Maslov index is determined entirely by the structure of $G(\mathbf{x}, \mathbf{x}', E)$ itself, so we do not have to deal with the propagator. The theory of multidimensional WKB approximations was greatly advanced by Maslov[6,7] and it is his approach that we follow in this paper. In the following subsection we give a brief description of WKB according to Maslov; more complete discussions can be found in Maslov,[6] Maslov and Fedoriuk,[7] Delos[8] or Percival.[9]

We would like to point out that a method has been derived by Möhring, Levit and Smilansky,[10,11] in which the Maslov index is determined directly for the energy-dependent Green's function. They write the energy-dependent Green's function as a Laplace transform of the path integral. Evaluating the integrals by the stationary phase approximation, they obtain Eq. (2.1.3) with explicit rules for determining the Maslov index. Such an approach is not suitable for our purposes however because it obscures the underlying geometry that we wish to examine in this paper. We will therefore proceed with Maslov's approach.

2.2 Some elements of multidimensional WKB theory

Within the WKB approximation a wavefunction is determined by a Lagrangian manifold L (giving the phase of the wavefunction) along with a particle density ρ (giving the amplitude) and a choice of overall phase. The reader who is not familiar with Lagrangian manifolds is referred to references 5,6 and 8. Heuristically we can think of the wavefunction as being represented by a collection of particles distributed over L with the density ρ. If we want to look at the wavefunction in, say, the x-representation we use the following action function,

$$S(l) = \int_\gamma \mathbf{p} \cdot d\mathbf{x}, \tag{2.2.1}$$

where γ is a path on L starting at some reference point l_0 on L and ending at l on L. Because L is Lagrangian, $S(l)$ does not change under continuous deformations of γ. This is why we can omit reference to γ in $S(l)$. To find the wavefunction $\psi(\mathbf{x}_0)$ at a given point $\mathbf{x}_0$ in configuration space we add up contributions from all the points l in L for which $\mathbf{x} = \mathbf{x}_0$. These will generally be discrete in number so we label them with the discrete index b. The wavefunction is

$$\psi(\mathbf{x}) = \sum_b |\rho(\mathbf{x})|^{\frac{1}{2}} \, e^{\frac{i}{\hbar} S(\mathbf{x}) - i\mu\pi/2}, \tag{2.2.2}$$

where $\rho(\mathbf{x})$ is the particle density in configuration space and μ is the Maslov index. The density $\rho(\mathbf{x})$ diverges at configuration space caustics where L has a singular projection onto configuration space as two branches of L coalesce (see Fig. (1)). At these points the WKB approximation breaks down in the x-representation. It can be shown however that there always exists a p- or mixed x-p-representation in which the wavefunction is caustic-free. In order that the wavefunction be smooth in these representations the Maslov index must differ between the two branches of the configuration space representation according to the following prescription.

First we find a good representation for the wavefunction at the $\mathbf{x}$-space caustic. A representation $(x_1, \cdots, x_k, p_{k+1}, \cdots, p_N)$ is good if the Lagrangian manifold has a non-singular projection onto the $(x_1, \cdots, x_k, p_{k+1}, \cdots, p_N)$ plane or, equivelently, if $(x_1, \cdots, x_k, p_{k+1}, \cdots, p_N)$ are good coordinates for the Lagrangian manifold. Then

we construct the following symmetric matrix R representing the linearised projection from L to configuration space

$$R = \frac{\partial(x_{k+1}, \cdots, x_N)}{\partial(p_{k+1}, \cdots, p_N)}. \tag{2.2.3}$$

On passing through a caustic the projection becomes singular and one or more eigenvalues of R passes through 0. The Maslov index is incremented by 1 for every eigenvalue of R that goes from negative to positive and is decremented by 1 for every eigenvalue going from positive to negative. This rule for the change in μ follows in a straightforward manner from performing the change of representation explicitly, using a stationary phase approximation. Usually we expect that every representation except the x-representation is good and that only one eigenvalue of R passes through 0.

As described above, this procedure for determining μ, which is the one most directly suggested by the change of representation, is mostly algebraic. It can be thought of however, in a way that is much more suggestive of the geometry, as arising from following the tangent plane to L as it rotates around in phase space on going from one point on L to another. On passing through a caustic the plane momentarily intersects momentum space non-trivially, typically along a 1-dimensional subspace, though at exceptional points this dimensionality may be higher. The change in signature of R then measures the 'sense' in which the plane passes through momentum space.

Let us illustrate this in the special case of a phase space of one degree of freedom. In this case any one-dimensional curve is a Lagrangian manifold and any one-dimensional subspace (*i.e.*, line) a Lagrangian plane. R is just a number, $\partial x/\partial p$, so let us denote it by r instead. It is easy to see that r is positive for any line just slightly counter-clockwise of the momentum axis and negative for a line just slightly clockwise of it. Therefore the Maslov index is incremented by one every time the tangent plane passes through the momentum axis in the clockwise sense and decremented by one every time it passes through in the counterclockwise sense. The total change in the Maslov index over a whole curve is just the clockwise intersection number of the tangent plane with the momentum axis, *i.e.*, the number of clockwise crossings minus the number of counterclockwise crossings.

It turns out that this particularly simple picture of the Maslov index in one degree of freedom is all we need for the periodic orbit sum of a two degree of freedom system if we use a reduction of the dynamics to surfaces of section. In the following section we outline how this is done for the Maslov index of the Green's function.

3. The energy-dependent Green's function and its Maslov index

We will consider $G(\mathbf{x}, \mathbf{x}', E)$ as a wavefunction in $\mathbf{x}$, parameterised by $\mathbf{x}'$ and E. With this point of view we can construct $G(\mathbf{x}, \mathbf{x}', E)$, just as in the previous section, from a Lagrangian manifold L and a particle density that we need not worry about for the Maslov index. L is made up of all the trajectories originating from $\mathbf{x}'$ at energy E. We start with the $(N-1)$-dimensional initial surface $\{\mathbf{x} = \mathbf{x}', H = E\}$ and let it flow under H for positive time. In this process L is swept out (see Fig. (2)). One can show that this manifold is Lagrangian and that its action coincides with the action of the paths in Eq. (1.1.3), so it does indeed give the phase of $G(\mathbf{x}, \mathbf{x}', E)$. Our aim is to follow the tangent plane to L between $\mathbf{x}'$ and $\mathbf{x}$ to find μ.

Let us focus on the contribution of a particular path to $G(\mathbf{x}, \mathbf{x}', E)$. It is convenient to use the following configuration space coordinates centered on the trajectory, as originally introduced by Gutzwiller. The coordinates are $(\mathbf{y}, z)$ (which we will still denote collectively by $\mathbf{x}$), with the $N-1$ coordinates $\mathbf{y}$ transverse to the path in such a way that $\mathbf{y} = 0$ specifies the path and with z a coordinate along the path. Expressed in these coordinates the amplitude $D(\mathbf{x}, \mathbf{x}', E)$ takes on a particularly simple form,

$$D(\mathbf{x}, \mathbf{x}', E) = \frac{1}{|\dot{z}\dot{z}'|^{\frac{1}{2}}} \left| \frac{\partial^2 S}{\partial \mathbf{y} \partial \mathbf{y}'} \right|^{\frac{1}{2}}, \tag{3.1}$$

as originally shown by Gutzwiller.[1] It was assumed by Gutzwiller in his original derivation of the trace formula that the coordinates $(\mathbf{y}, z)$ were orthogonal. It turns out however, that this assumption is not necessary; the derivation follows through, with minor modifications, for any set of coordinates constructed from the trajectory in this way, irrespective of whether they are orthogonal. This is a reflection of the fact that the only relevant structure on phase space should be its symplectic

structure; any metric properties of configuration space should not affect the final results. It also turns out that for Eq. (3.1) to hold, it is not even necessary for $(\mathbf{y}, z)$ to be tied to the orbit; they can be arbitrary coordinates on configuration space.[12] However, for our purposes it will suffice to apply this formula to path-centered coordinates.

Caustics are signalled by a divergence of the amplitude in Eq. (3.1), of which there are two types. The first occurs when $\dot{z} = 0$ (which implies that $\dot{\mathbf{x}} = 0$). In this case the trajectory stops and forms a cusp in configuration space as it moves from one branch of L to another(Fig. 3(b)). (A special case, which often occurs in practice, is when the trajectory retraces its path in configuration space. We will also refer to this occurance as being a cusp.) This type of caustic is the only possibility in one degree of freedom, where a trajectory is obliged to retrace its path. Cusps should not be expected to appear in higher dimensional systems for generic Hamiltonians. However, periodic orbits of kinetic-plus-potential Hamiltonians do exhibit cusps (in which the trajectory retraces its path), because of time reversal symmetry, and therefore orbits with cusps are quite common in applications.

The second type of caustic occurs when $|\partial^2 S/\partial \mathbf{y} \partial \mathbf{y}'|$ diverges. In more than one degree of freedom this is the most common case and corresponds to the trajectory moving between branches of L in configuration space without stopping.

We will deal only with the second case. If the first case arises and the trajectory forms a cusp in configuration space at the caustic, we can treat it as if there were no cusp by doing the analysis in the momentum represention. While the intermediate results will be different, the final conclusions about the Maslov index in the trace formula will be independent of representation. The reason we want to avoid cusps is that when they occur the coordinates $(\mathbf{y}, z)$ constructed above are ill-defined, as are the surfaces of section and their mappings that we will consider presently.

Let us refer to the set of points in configuration space that correspond to caustics of L as the 'caustic surface'. Apart from exceptional singular points the caustic surface is a simple $(N-1)$-dimensional surface. The caustic crossings that we are considering are such that the trajectory approaches the caustic surface, touches it tangentially and moves away again. This means that the z direction is tangent

to the caustic surface at the crossing. It is shown in appendix A that this implies a good representation for the Green's function at the caustic can always be found by choosing z and some combination of the y's and p_y's, *i.e.*, that we never have to change representation in the z component. It is this fact that allows us to determine the Maslov index by working entirely with the dynamics in surfaces of section that we construct as follows.

At each point z_0 along the trajectory we denote by $\Sigma(z_0)$ the surface of section formed by the set $\{z = z_0, H = E\}$. We use $(\mathbf{y}, \mathbf{p}_y)$ as canonical coordinates on $\Sigma(z_0)$. Between any two surfaces of section, $\Sigma(z')$ and $\Sigma(z)$ say, we can construct a symplectic surface of section mapping $F(z, z')$. By letting z vary continuously $F(z, z')$ can be regarded as a Hamiltonian flow in 'time' z, one slight complication being that the space in which the flow takes place, $\Sigma(z)$, is changing continually as one moves forward in z. The linearisation of $F(z, z')$ about the reference trajectory, $M(z, z')$, is a $(2N-2) \times (2N-2)$ symplectic matrix which we write in block form as,

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{3.2}$$

so that we have explicitly for initial and final variations $(\delta\mathbf{y}', \delta\mathbf{p}'_y)$ and $(\delta\mathbf{y}, \delta\mathbf{p}_y)$, respectively,

$$\delta\mathbf{y} = A\delta\mathbf{y}' + B\delta\mathbf{p}'_y, \tag{3.3a}$$

$$\delta\mathbf{p}_y = C\delta\mathbf{y}' + D\delta\mathbf{p}'_y. \tag{3.3b}$$

The surfaces of section and their mappings are useful because the Jacobian matrices R of Eq. (2.2.3) that are used to determine the Maslov index are all taken at constant z for the representations that we are considering and so are derivatives along the surfaces of section. As a consequence, they can be written in terms of M and its elements. Suppose for example that a good representation is $(z, \mathbf{p}_y)$, as it will be in most cases. Then μ is determined by the change in signature of the matrix,

$$R = \frac{\partial \mathbf{y}}{\partial \mathbf{p}_y} = BD^{-1}, \tag{3.4}$$

where the second equality follows easily from Eq. (3.3). The case of more general representations such as $(z, y_1, \cdots, y_k, p_{y_{k+1}}, \cdots, p_{y_{N-1}})$, can be dealt with by manip-

ulating submatrices of BD^{-1}. Caustic crossings occur precisely when B becomes singular. This is evident from Eq. (3.4) in the case of typical crossings, but is actually true in general, even when $(z, \mathbf{p}_y)$ is not a good representation. Physically, if ξ is a null eigenvector of B, then an initial pencil of rays, emerging from $\mathbf{x}'$ with $(\delta\mathbf{y}', \delta\mathbf{p}'_y)$ proportional to the vector $(0, \xi)$, refocusses at the caustic where $(\delta\mathbf{y}, \delta\mathbf{p}_y)$ is proportional to $(B\xi, D\xi) = (0, D\xi)$.

One should note that the initial point of any trajectory lies right on top of a highly degenerate caustic for which $M = I$ and therefore $R = BD^{-1} = 0$. Because the trajectory starts on this caustic and does not actually pass through it one needs to give it special consideration. The increment in μ that one assigns to this initial caustic is determined as follows: μ receives an increment of 1 for every negative eigenvalue of $R(0^+)$, where $R(0^+)$ denotes the R-matrix constructed for infinitesimally short times along the orbit. For example if all the eigenvalues of R are initially positive (as discussed in appendix B, this is always the case for kinetic plus potential systems) then $\mu = 0$ initially. It is helpful to note that μ is determined from this initial caustic as if all of the eigenvalues of R were initially infinitesimally positive and the trajectory went cleanly through the caustic.

One can see that the initial value of μ is determined in this way by considering the propagator for short times. In a momentum representation the WKB approximation for the propagator is not ambiguous at $t = 0$ and in fact can be written $K(\mathbf{p}, \mathbf{x}', t = 0) = (2\pi\hbar)^{N/2}\exp(-i\mathbf{p} \cdot \mathbf{x}')$. In transforming to a position representation for short but nonzero times one finds that the initial value of the Maslov index of the propagator is determined by its Lagrangian manifold according to rules similar to those outlined above for the energy-dependent Green's function. If the energy-dependent Green's function is then computed from the propagator by means of a Laplace transform in time, the stated procedure for finding the initial Maslov index of the energy-dependent Green's function is recovered.

Therefore we have the following algorithm for determining the Maslov index of the energy-dependent Green's function. First we construct, all along the trajectory from $\mathbf{x}'$ to $\mathbf{x}$, the surfaces of section $\Sigma(z)$. From them, we find the surface of section mappings and their linearisations M. Next, we find those places along the trajectory at which the component B of M is singular; these are the caustics. Finally, at

each caustic, we add a contribution to μ according to the signature change of the symmetric matrix, BD^{-1}. In particular one increments μ by one for every negative eigenvalue of BD^{-1} computed for short times.

We can view this procedure in a way that is directly connected with the discussion of the previous section, concerning the determination of Maslov indices from the evolution of Lagrangian planes. Here however, rather than finding the Maslov index from the evolution of N-dimensional Lagrangian subspaces of the $2N$-dimensional phase space, we find the index from the evolution of $(N-1)$-dimensional Lagrangian subspaces of the $(2N-2)$-dimensional surfaces of section. The $(N-1)$-dimensional subspaces we speak of are the tangent planes of the intersection of L with the surfaces of section, at the trajectory. The intersection of L with the surface of section $\Sigma(z')$, at the start of the trajectory, coincides with the $(N-1)$-dimensional momentum space of $\Sigma(z)$, which we denote by $P(z')$. The intersection with the surface of section $\Sigma(z)$, at some later point of the trajectory, is obtained by letting $P(z')$ flow forward under $F(z,z')$, giving $F(z,z')P(z')$. Linearising about the trajectory, we find that L intersects $\Sigma(z)$ along the $(N-1)$-dimensional plane $M(z,z')P(z')$, which we denote by $\lambda(z)$. (M is defined by Eq. (3.3).) At caustics, where B is singular, we find that $\lambda(z)$ intersects $P(z)$ nontrivially, along $(B\xi, D\xi) = (0, D\xi)$, where ξ is the null eigenvector of B. As $\lambda(z)$ passes through $P(z)$, μ is incremented according to the sense in which it passes through, as determined by the change in signature of BD^{-1}. Evidently, we determine μ from the evolution of $\lambda(z)$ in $\Sigma(z)$ in exactly the same way that we would determine the index of an $(N-1)$-dimensional wavefunction propagating in time, by following the tangent plane to its Lagrangian manifold in the phase space of $(N-1)$-degrees of freedom.

By passing to the surface of section dynamics, we have essentially achieved a reduction in the number of degrees of freedom, at least as far as the Maslov index is concerned. This is a useful picture for determining the geometrical properties of σ, and it is the point of view we will adopt in the forthcoming sections. In applications however, for example if one wanted to numerically analyse the trace formula for a kinetic-plus-potential system, it might be better to use a method which does not depend on the construction of the $(\mathbf{y}, z)$ coordinates and the surfaces of section $\Sigma(z)$. We outline how this can be done in appendix B.

Finally we note that the prefactor $\left|\partial^2 S/\partial \mathbf{y}\partial \mathbf{y}'\right|^{\frac{1}{2}}$ can be written very simply in terms of the surface of section mappings. Using the generating function conditions on $S(\mathbf{x},\mathbf{x}',E)$, we can write $\partial^2 S/\partial \mathbf{y}\partial \mathbf{y}' = -\partial \mathbf{p}'_y/\partial \mathbf{y}$, which is equal to $-B^{-1}$ and so we can write the Green's function as,

$$G(\mathbf{x},\mathbf{x}',E) \approx \frac{1}{i\hbar}\frac{1}{(2\pi i\hbar)^{(N-1)/2}}\sum \frac{\exp\left(\frac{i}{\hbar}S(\mathbf{x},\mathbf{x}',E) - i\mu\pi/2\right)}{\left|\dot{z}\dot{z}'\det B\right|^{\frac{1}{2}}}. \tag{3.6}$$

This completes the discussion on the Green's function. The next step for the trace formula is to actually take the trace. This introduces extra contributions to the Maslov index that we describe in the next section.

4. The determination of σ

In this section we discuss the index of the trace formula as it arises in performing the trace in Eq. (1.1.1). In 4.1 we show how σ arises in taking the trace and in 4.2 we examine the question of whether the σ is constant along an orbit.

4.1 Taking the trace

Now let us proceed with evaluating the trace,

$$\mathrm{Tr}\, G = \int d\mathbf{x}\, G(\mathbf{x},\mathbf{x},E), \tag{4.1.1}$$

where $G(\mathbf{x},\mathbf{x},E)$ is written as a sum over trajectories $\mathbf{x} \to \mathbf{x}$, *i.e.*, trajectories that close in $\mathbf{x}$-space. We follow here the original derivation of Gutzwiller.[1] Doing the integral by the stationary phase approximation yields contributions from the periodic orbits, *i.e.*, those trajectories that close in the full phase space. In the neighbourhood of each periodic orbit, we find that the integral over $\mathbf{x}$ splits up into an integral in z along the orbit and one in $\mathbf{y}$ transverse to the orbit.

The integral in $\mathbf{y}$ is a complex gaussian

$$I_\perp = \int d\mathbf{y} \exp\Big(\frac{i}{2\hbar}\tilde{\mathbf{y}}\frac{\partial^2 S(\mathbf{x},\mathbf{x},E)}{\partial \mathbf{y}\partial \mathbf{y}}\mathbf{y}\Big). \tag{4.1.2}$$

Where $\tilde{\mathbf{y}}$ is the transpose of $\mathbf{y}$. The matrix $W \equiv \dfrac{\partial^2 S(\mathbf{x},\mathbf{x},E)}{\partial \mathbf{y}\partial \mathbf{y}}$ can be written as

$$\left(\frac{\partial^2 S(\mathbf{x},\mathbf{x}',E)}{\partial \mathbf{y}'\partial \mathbf{y}'} + \frac{\partial^2 S(\mathbf{x},\mathbf{x}',E)}{\partial \mathbf{y}\partial \mathbf{y}'} + \frac{\partial^2 S(\mathbf{x},\mathbf{x}',E)}{\partial \mathbf{y}'\partial \mathbf{y}} + \frac{\partial^2 S(\mathbf{x},\mathbf{x}',E)}{\partial \mathbf{y}\partial \mathbf{y}}\right)_{\mathbf{x}=\mathbf{x}'}, \quad (4.1.3)$$

which, using the generating function conditions on $S(\mathbf{x},\mathbf{x}',E)$, can be reduced to

$$W = B^{-1}A - B^{-1} - \tilde{B}^{-1} + DB^{-1}, \quad (4.1.4)$$

where these matrices are derived from the surface of section mapping taken once fully around the periodic orbit. (We would like to emphasise that this is not quite the same as before. Until now we have considered mappings between different points on the orbit.) The transverse integral is then

$$I_\perp = \frac{(2\pi i\hbar)^{\frac{(N-1)}{2}}}{|\det W|^{\frac{1}{2}}} e^{i\nu\pi/2},$$

where the index ν is the number of negative eigenvalues of W. This combines with μ, the Maslov index of the Green's function, to give the index, σ of the trace formula, *i.e.*,

$$\sigma = \mu + \nu. \quad (4.1.5)$$

We are now left with just the longitudinal z integral and the sum, after some manipulation, reduces to

$$\mathrm{Tr}\, G = \frac{1}{i\hbar} \sum_{\text{po's}} \oint dt \, \frac{\exp\left(\frac{i}{\hbar}S - i\sigma\pi/2\right)}{|\det(M-I)|^{\frac{1}{2}}}, \quad (4.1.6)$$

where dt is the time increment $dz/\dot{z}$ (we assume that z is defined in such a direction that $\dot{z} > 0$) and $\oint$ denotes an integral around a single iteration of the primitive orbit.

It is customary at this stage of the calculation to note that the integrand is constant and to replace $\oint$ with T, the period of the primitive orbit. However we would like to raise the objection that it is not completely obvious that σ is constant around the orbit, though this seems very natural and ultimately turns out to be true. We will examine this question in 4.2.

4.2 Is the index constant?

In previous discussions of the trace formula it has often been implicitly assumed that the index σ can be obtained by counting caustics of the energy-dependent Green's function, or even the time-dependent Green's function $K(\mathbf{x},\mathbf{x}',t)$. It is important to realise that this is not true. A count of caustics yields μ which depends, for its definition, on having a preferred set of coordinates in phase space, namely those connected with the x-representation in which we compute the Green's function. It should not determine completely something that should be a phase space invariant like the index of the trace formula.

In fact, μ is not even a property of the orbit since it can depend on the starting point of the orbit. We illustrate this with a specific example from the stadium billiard.[13,14] In Fig. (6) we show an orbit which, depending on the starting point, can have either one or two caustics. The μ that we calculate with each of these starting points will be different; it will be greater by one for the starting point with two caustics. A more detailed analysis of the same orbit would reveal that ν is also different for these two starting points.

Therefore we see that neither μ nor ν is an intrinsic property of the orbit alone; each depends on where we start the orbit. How is it then that their sum $\sigma = \mu + \nu$ depends only on the orbit? Obviously it must be that they both change at the same places on the orbit and change there by equal and opposite amounts.

The index ν changes at those points at which an eigenvalue of W changes sign, either by going through 0 or by going through infinity. We note the following identity that is used in deriving the trace formula:

$$\det W = (-1)^N \frac{\det(M-I)}{\det B}. \tag{4.2.1}$$

Since $\det(M-I)$ is an invariant of the orbit and in particular never changes sign, we see that an eigenvalue of W changes sign at precisely those points at which B (computed for a full iteration of the orbit) is singular and does so by going through infinity. But it is at these points that μ changes also. If B is singular a caustic lies right on top of the initial/final point of the orbit. If we shift this point a little then the caustic will move relative to it. According to whether the orbit closes before

or after the trajectory crosses the caustic, a different number of caustics crossings and therefore a different Maslov index μ will be assigned to the orbit. A convenient terminology is to call points at which a caustic lies on top of the initial/final point self-conjugate points. This terminology has been used by Bogomolny[15] and Heller.

Therefore since both μ and ν change at the same points it is possible that they change in such a way that σ is constant. It is easy to demonstrate this explicitly, at least in two degrees of freedom, but we will not do it here since it will become completely transparent once an interpretation for σ as a winding number of the stable and unstable manifolds has been developed. For now we note that σ is indeed constant and write the trace formula as

$$\mathrm{Tr}\, G = \frac{1}{i\hbar} \sum_{\text{po's}} \frac{T}{|\det(M-I)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}S - i\sigma\pi/2}. \tag{4.2.2}$$

Here, the period T refers to the primitive orbit, whereas S and M refer to the full orbit. In the next section we will pursue the the geometrical aspects of σ.

5. Geometrical interpretation for σ

Let us now restrict ourselves to the special case of unstable orbits in systems of two degrees of freedom. For these systems, the dimensions of the objects we are considering are low enough that we can easily visualise them. We show in this section, using geometrical arguments, that the index σ for these systems is twice the clockwise rotation number of the stable and unstable manifolds around the periodic orbit in the surfaces of section $\Sigma(z)$.

5.1 σ is a winding number

First we observe that for systems of two degrees of freedom the surfaces of section are two-dimensional, embedded in the three-dimensional energy shell $H = E$. The linearised surface of section mapping M, between any two surfaces of section, is a 2×2 matrix so let us denote it by

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{5.1.1}$$

The Lagrangian manifold L, associated with the energy-dependent Green's function, is also a two-dimensional surface in the energy shell and intersects each surface of section $\Sigma(z)$ along a one-dimensional curve. In the notation of Sec. 3 this curve is tangent to the line $\lambda(z)$ at the orbit (see Fig. (5)). We obtain $\lambda(z)$ by mapping the momentum axis of $\Sigma(z')$ forward with $M(z, z')$ Therefore it is the line spanned by the vector (b, d).

Because the surfaces of section $\Sigma(z)$ are 2-dimensional and the lines $\lambda(z)$ are 1-dimensional, it is easy to find μ. We just follow $\lambda = \text{span}(b, d)$ as it rotates around in the surfaces of section. Then μ is the clockwise intersection number of λ with the momentum axis, just as described for a system of one degree of freedom in Sec. 2.2. That is, we increment μ by one for every clockwise intersection of λ or (b, d) with the momentum axis and decrement it by one for every counterclockwise intersection.

Having rotated around in the surfaces of section $\Sigma(z)$, the line λ finally ends up in a direction that is determined by the surface of section matrix M of a full iteration of the periodic orbit. Because the orbit is unstable M will have a hyperbolic structure that places *a priori* restrictions on the final direction of λ (Fig. (7)). More precisely, M has two real eigenvectors, e_u and e_s say, corresponding to real eigenvalues τ and $1/\tau$ respectively, where $|\tau| > 1$. The vectors e_u and e_s are tangent to the unstable and stable manifolds at the orbit. These directions divide the surface of section into four quadrants, which we label H, I, J, K, starting clockwise from H, containing the upper momentum axis (see Fig.(8)). It is not difficult to see that, according as M is hyperbolic ($\tau > 0$) or hyperbolic with reflection ($\tau < 0$), the vector (b, d) ends up in either the same quadrant as it started in, H, or the opposite

one, J. Similarly the line λ, which starts out running through the pair of opposing quadrants H and J, must end up in the same pair of quadrants.

The index ν depends very simply on where λ finally ends up within the quadrants H and J. First we recall that $\nu = 0$ if $w \equiv (a+d-2)/b$ is positive and $\nu = 1$ if w is negative. Next we note that

$$w = \frac{a+d-2}{b} = \frac{\mathrm{Tr}\, M - 2}{b} = \frac{\tau + 1/\tau - 2}{b}. \tag{5.1.2}$$

Since $|\tau + 1/\tau| > 2$ we conclude that $\tau + 1/\tau - 2$ has the same sign as $\tau + 1/\tau$ and therefore τ. This means that the numerator of w is positive if M is hyperbolic and negative if M is hyperbolic with reflection. The denominator, b, is positive or negative according as the vector ends up to the right or the left of the momentum axis. Let us further divide the quadrants H and J into the sectors H_-, H_+, J_- and J_+ as shown in Fig. (8). The $-$ subscripts indicate the sectors that are clockwise of the momentum axis and the $+$ subscripts indicate the sectors that are counterclockwise of it. Then we find that w is positive if the vector (b, d) ends up clockwise of the momentum axis, in either of the sectors H_+ or J_+, (τ and b have the same sign) and is negative if (b, d) ends up counterclockwise of it, in either of the sectors H_- or J_- (τ and b have opposite signs). Equivalently, $\nu = 0$ if λ ends up running through the sectors H_+ and J_+, and $\nu = 1$ if λ ends up running through the sectors H_- and J_-.

Having found the geometrical meanings of μ and ν, we next examine their sum σ. With an appropriate generalisation of the sectors H, I, J, K to surfaces of section at intermediate points along the orbit, we will show that, whereas μ is the net number of times that λ passes through the momentum axis, σ is the net number of times that λ passes through either of the sectors I and K.

The sectors H, I, *etc.* are defined by the eigenvectors e_s and e_u of the surface of section mapping for a specific surface of section $\Sigma(z')$. We can extend them from this initial surface of section to intermediate surfaces of section by extending the vectors e_s and e_u. We do this by constructing the vectors $e_u^*(z)$ and $e_s^*(z)$ in $\Sigma(z)$, which are given the same coordinates relative to the y and p_y axes in $\Sigma(z)$ as e_u and e_s have in $\Sigma(z')$. That is, moving around the periodic orbit, $e_s^*(z)$ and

$e_u^*(z)$ (and therefore the sectors H, I, *etc.*) are held rigid with respect to the y and p_y axes. We would like to stress that this is neither the most obvious nor the most natural extension of e_s and e_u. The only intrinsically meaningful way to extend e_s and e_u is to map them forward with the surface of section mappings. The vectors $e_u(z) = M(z,z')e_u(z')$ and $e_s(z) = M(z,z')e_s(z')$ defined in this way are just the the stable and unstable directions of the intermediate surface of section $\Sigma(z)$. While $e_u(z)$ and $e_s(z)$ are defined independently of any coordinate systems that we might choose, the vectors $e_u^*(z)$ and $e_s^*(z)$ depend, for their definition, on having the preferred coordinate systems y-p_y in the surfaces of section $\Sigma(z)$. Such non-invariant quantities can be significant however in determining μ and ν because μ and ν are in turn coordinate-dependent quantities.

As we follow λ around the orbit we can define μ for intermediate points, before the orbit closes. It is the net number of clockwise intersections of λ with the momentum axis up to that point. We cannot, strictly speaking, do the same for ν (and therefore σ) as it is defined only in terms of the surface of section matrix for the completed orbit. However, with the aforementioned definition of the sectors H, I, *etc.* for points on the periodic orbit other than the initial point, we can artificially define ν for these intermediate points, according to the positioning of λ relative to H, I, *etc.* We define ν to be 0 if λ is clockwise of the momentum axis, in the sectors H_+ and J_+, and 1 if λ is counterclockwise of it, in the sectors H_- and J_-. We will not bother to define ν for λ in the other two quadrants, I and K, because λ will not be in them at the end of the trajectory.

With this extension of ν to intermediate points, σ varies very simply as λ evolves in the surfaces of section. It is clear that as λ sweeps through quadrants H and J, σ remains unchanged, the change in ν exactly compensating for the change in μ whenever λ passes through the momentum axis. On the other hand, σ changes by one every time λ passes completely through the quadrants I and K. In fact, taken over the whole orbit, σ is the clockwise intersection number of λ with the quadrants I and K.

We can state this even more simply in terms of the stable and unstable manifolds. First let us stress the following rather obvious fact: if λ does not coincide with any of the invariant manifolds at the initial point, it cannot coincide with them

at any other point along the orbit. This is because M, being symplectic, can never be singular and so cannot map two distinct directions into one. This implies that λ sweeps the invariant manifolds along with it as it rotates around in the surfaces of section. Therefore the invariant manifolds have the same intersection number with the sectors I and K that λ has. This intersection number is especially significant for the invariant manifolds because they have the property that they return to themselves on going once fully around the orbit. Because they return to themselves they rotate around in the surfaces of section some half-integer number of times, a half-rotation being equal to a rotation of 180^0. We can count the number of clockwise rotations using the intersections with the quadrants I and K: between every clockwise half-rotation there is a single clockwise intersection with I and K. Therefore the net number of clockwise half-rotations is equal to the net clockwise intersection number with I and K. This implies that σ is precisely twice the number of times the invariant manifolds rotate around the periodic orbit in the clockwise direction. This is the principal result of this paper.

We wish to point out that, since the space in which the winding number is defined is changing throughout the loop, there is no *a priori* fixed frame relative to which the winding number is measured. Instead, the winding number is obtained from the rotation relative to the set of y-p_y axes in succesive surfaces of section. (We showed above that it was measured relative to the quadrants H, I, *etc*, but by definition these are held fixed relative to the y-p_y frame.) This is characteristic of all Maslov indices; they need, for their definition, a global coordinate system to exist on phase space, which in this case corresponds to the (y, z, p_y, p_z) coordinates around the orbit.

We can generalise the definition of the winding number to be independent of the (y, p_y) as follows. We measure the winding number relative to any continuous and periodic set of vectors $e(z)$ in the surfaces of section $\Sigma(z)$ which has the property that the Lagrangian planes spanned by $e(z)$ and the flow vector of the Hamiltonian have a zero Maslov index on going once around the periodic orbit. The justification for this comes when we show in a later section, by lifting the calculation from the surfaces of section to the full phase space, that σ is actually given by the rotation of the two dimensional invariant manifolds relative to the p-x frame. In doing this

we remove all reference to the choice of y and z as configuration space coordinates. In fact σ is computed from the invariant manifolds in exactly the same way that we compute for example, the Maslov index of invariant tori in torus quantisation. In this sense σ is truly a Maslov index.

5.2 Remarks

With this interpretation of σ as a winding number of the invariant manifolds a number of facts become obvious that are not at all clear if we simply regard σ as being the sum of μ and ν.

First it is now obvious that σ does not depend on the starting point on the orbit, since the number of times the invariant manifolds wind around is the same no matter where we start. We were therefore justified in replacing $\oint dt$ by T in Eq. (4.1.6).

Next we observe that if the orbit is iterated more than once, σ scales directly with the number of iterations, that is, if σ_0 is the index of a primitive orbit, σ increments by σ_0 for every successive iteration of it. This is a trivial consequence of the fact that σ is a winding number; the invariant manifolds make σ_0 half-rotations during each iteration of the primitive orbit, independently of the history of the orbit. This property of σ is *not* obvious from $\sigma = \mu + \nu$ because neither μ nor ν scales with the number of iterations. The contributions μ and ν do not increment by the same amount in each iteration because each of them depends on the history of the orbit. For example μ is determined by the refocussing of a pencil of trajectories emerging from the initial point $\mathbf{x}'$ of the first iteration of the primitive orbit. These trajectories will refocus at different places along, say, the second iteration of the primitive orbit than they did in the first because the trajectories starting the second iteration will already have been dispersed on passing through the primitive orbit the first time. In particular there is no reason why there should even be the same number of caustics in each iteration. For example, in the orbit of Fig. (6(a)) there is just one caustic in the first iteration whereas two caustics will occur in a second iteration of the same orbit. Just as μ does not scale with the number of iterations so it is that ν does not scale with the number of iterations either. This is obvious because ν can only

be 0 or 1 and cannot therefore increase indefinitely. Since neither μ nor ν scales with the number of iterations it is not easy to see directly that their sum $\sigma = \mu + \nu$ does, this becomes apparent only after we realise that σ is a winding number. In fact, to our knowledge, there has not been a proof of this fact until now, though in previous discussions of the trace formula it has been taken for granted that this is the case.

Finally we note that σ is odd if and only if the orbit is hyperbolic with reflection. σ is odd precisely when the invariant manifolds make some half-integer number of rotations. In this case a vector, e say, along an invariant manifold ends up, on being propagated once around the orbit, pointing in the opposite direction to the one in which it started. Clearly this is the case if and only if the orbit is hyperbolic with reflection. The fact that σ can be odd for orbits that are hyperbolic with reflection is a direct consequence of the non-orientability of the invariant manifolds of such orbits. These invariant manifolds are like two-dimensional strips that have an odd number of twists put in them and which are then glued at the ends, so topologically they are like Möbius strips. It can be shown[16] that Maslov indices defined for closed curves on a Lagrangian manifold can be odd only if the the Lagrangian manifold is non-orientable. In the next section we show how σ is a Maslov index defined in the usual way by the invariant manifolds.

6. Extensions and further observations

In this section we will explore some of the ramifications of the results derived in the previous section. In 6.1 we examine how σ may be interpreted in the full phase space and in 6.2 we show that σ may be regarded as the winding number of the periodic orbit.

6.1 σ as a Maslov index in the full phase space

In Sec. 3 we showed how the Maslov index of the energy-dependent Green's function, μ, could be found by following the Lagrangian manifold, L, in the surfaces of section. In this section we go in the opposite direction. That is, we lift σ from the surfaces of section to show that it is the Maslov index of the invariant manifolds, defined in the full phase space. For notational convenience we will often refer only to the unstable manifold in what follows, everything we say about the unstable manifold will hold equally well for the stable manifold.

As we have noted already, the unstable manifold is a two-dimensional Lagrangian manifold that intersects each surface of section $\Sigma(z)$ along a one dimensional curve that is tangent to the vector $e_u(z)$ at the periodic orbit. Its Maslov index along any closed curve, such as the periodic orbit that defines it, is determined by the rotation of the two-dimensional tangent plane in the four-dimensional phase space relative to the momentum plane. The Maslov index receives a contribution every time the tangent plane passes through momentum space, just as described in Sec. 2. We could determine the Maslov index along the periodic orbit, just as we determined the Maslov index of the energy-dependent Green's function in Sec. 3, by dealing with the caustics in the (z, p_y) representation. This would lead to the prescription of following the unstable manifold in the surfaces of section: the Maslov index is the number of clockwise intersections of the tangent vector to the unstable manifold, $e_u(z)$, with the p_y axis of $\Sigma(z)$ minus the number of counterclockwise intersections. This is *exactly* the prescription we found in the previous section for determining σ. Therefore σ is the Maslov index of the unstable (and stable) manifold taken around the periodic orbit.

One might well ask why it is useful to know that σ is a Maslov index in the full phase space. This interpretation is certainly more complicated computationally than the surface of section picture, since we need to deal with a phase space of two degrees of freedom rather than the one degree of freedom of the surfaces of section. One reason it is useful is that, when we regard σ as a Maslov index of the invariant manifolds, it is not tied up with any particular set of coodinates, such as the (y, z, p_y, p_z) coordinates, or any unnecessary phase space structures, such as the

surfaces of section $\Sigma(z)$, which we would need otherwise. For example, caustics that occur at configuration space cusps are difficult to deal with in the surface of section picture because the coordinates (y, z, p_y, p_z) break down there, but are easily dealt with in the full phase space picture since we are free to choose any configuration space coordinates (x_1, x_2) along with their momenta (p_1, p_2), in examining the caustic. Another reason is that the Maslov index is very well understood and an extensive theory exists for it that we can apply to σ. For example it was possible in the previous section to observe that odd σ can exist for orbits that are hyperbolic with reflection only because their invariant manifolds are non-orientible.

One can also see that, for Hamiltonians of the form kinetic plus potential, it is possible to determine σ from a simple count of the caustics of the invariant manifolds. (More generally it can be shown[5,10,11] that the Maslov index defined by any Lagrangian manifold which evolves under the flow of a kinetic-plus-potential Hamiltonian increases along trajectories.) The caustics of the invariant manifolds correspond precisely to the self-conjugate points; every self-conjugate point is on a caustic of either the stable or the unstable manifold, and vice versa. The number of self-conjugate points is therefore equal to the number of caustics of the stable manifold plus the number of caustics of the unstable manifold. Therefore σ, which is equal to the number of caustics of either of the invariant manifolds, is equal to half the number of self-conjugate points. Similar observations have been made previously by Bogomolny.[15]

Finally, the fact that σ corresponds to the winding number of the invariant manifolds in the full phase space admits an immediate generalisation to higher dimensions. This generalisation, which follows from the application of a theorem of Arnol'd, is discussed in the next section.

6.2 Connection with Arnol'd's theory

The main result of Sec. (5), namely that in two dimensions the Maslov index in the trace formula is equal to the winding number of the invariant manifolds, admits a generalisation to higher dimensions. This follows from the observation, implicit in the preceding analysis, that an unstable periodic orbit has associated

to it, in a canonically invariant way, a winding number.[4] The argument is as follows. It is straightforward to show that the invariant manifolds of unstable orbits are Lagrangian, just as the KAM tori which surround stable orbits are Lagrangian. Therefore, an unstable periodic orbit may be regarded as a closed curve on a Lagrangian manifold.

Arnol'd has shown that the Maslov index of a closed curve on a Lagrangian manifold is an intrinsic property of the curve, and is a topogical invariant. The argument is based on associating to the original curve, $\gamma(t)$, a new curve $\lambda(t)$ in the abstract space of Lagrangian planes, which we denote by Λ. It turns out that Λ has a nontrivial topology, and in particular has the fundamental group of a circle. This means that one can choose in Λ a fundamental closed curve $\overline{\lambda}(t)$ that cannot be contracted to a point, so that any closed curve, such as $\lambda(t)$, can be continuously deformed into some number n of iterations of $\overline{\lambda}(t)$. Arnol'd has shown that n, the winding number of λ is precisely the Maslov index of $\gamma(t)$ (provided the sense of $\overline{\lambda}(t)$ is correctly chosen). This is because the set of Lagrangian planes that have nontrivial intersection with momentum space, C say, (these correspond to caustics), partition Λ in such a way that the intersection number of a closed curve with C (this is the Maslov index) is equal to the winding number of the curve.

It is easy to see how this works in one degree of freedom. Here phase space is a two-dimensional plane and the Lagrangian planes are precisely the one-dimensional subspaces. We can parameterise a Lagrangian plane λ by the angle ϕ it makes with the x-axis. ϕ ranges from 0 to π, and the angles 0 and π are identified, since they both correspond to the plane along the x-axis. Thus Λ can be mapped onto the unit circle according to $\lambda \rightarrow 2\phi$. (On the unit circle the angle ϕ increases counterclockwise according to the usual convention.) For the fundamental closed curve $\overline{\lambda}(t)$ we take a single clockwise winding of the unit circle. The Maslov index of of a curve $\lambda(t)$ is then given by the net number of times it passes through $\phi = \pi/2$ in the clockwise direction. For closed curves this is just equal to the number of clockwise windings. We have already seen that this is so in the case of the Maslov of the invariant manifolds when we follow them in the one degree of freedom surfaces of section.

The most familiar application of Arnol'd's theorem is in the torus (or EBK)

quantisation conditions, where the Maslov indices are the winding numbers of the tangent planes along the angle contours on invariant tori. Since unstable periodic orbits may also be regarded as closed curves on Lagrangian manifolds, they also have, according to Arnol'd's theorem, a winding number. This winding number is a canonical invariant, and is additive with the number of iterations of the orbit. It is natural to conjecture that in more than two dimensions, the index of the trace formula is still given by this winding number.

7. Conclusions

In this paper we have demonstrated that, in two degrees of freedom, the Maslov index appearing in the trace formula has a phase space invariant meaning as the Maslov index of the stable and unstable manifolds or, alternatively, as a winding number of the stable and unstable manifolds in surfaces of section (or even the full phase space, using Arnol'd's construction). In doing so we have placed the Maslov index on an equal footing with the other classical quantities appearing in the trace formula. These are the action of the orbit S, the period of the primitive orbit T and the quantity $\det(M - I)$ which is derived from the surface of section mapping M, all of which are invariant under canonical changes of coordinates in phase space.

That the invariance of the Maslov index is not obvious from the usual derivations of the trace formula is an unsatisfactory feature of these derivations. One would hope that it should be possible to derive the trace formula in such a way that its canonical invariance is obvious from the start. Such a derivation would hopefully be simpler and more transparent than the one discussed in this paper, which is the only one that has been presented to date. One of us[12] has in fact found a formulation in which trace formulas are found in a phase space invariant way. Hopefully this approach might lead to a more transparent demonstration of the facts presented in this paper.

While our arguments apply to two dimensions, it should be true in any number of dimensions that the Maslov index in the trace formula is an intrinsic property of the periodic orbits. We have conjectured that this index is the winding number of the invariant manifolds. This remains to be proved.

Appendix A

In this appendix we show that configuration space coordinates that run along the caustic surface at a caustic crossing can always be chosen to be part of a good representation at the caustic. In particular, this means that, for the coordinates (y, z) defined in Sec. 3, a good representation can always be found in which z rather than p_z is used. Because there is little added difficulty in doing so, we deal in this appendix with the more general case of configuration space coordinates $(x_1, \cdots, x_N)$, for which $(x_1, \cdots, x_k)$ are parallel to the caustic surface. In this case we want to show that a good representation can always be found in the form $(x_1, \cdots, x_k,\ x_{k+1} \text{ or } p_{k+1}, \cdots,\ x_N \text{ or } p_N)$. The proof of this is based on the following proposition.

Proposition: At a caustic, with configuration space coordinates $(x_1, \cdots, x_N)$ as described above, the tangent plane to the Lagrangian manifold that defines the caustic, intersects momentum space P along some subspace of the $p_{k+1}, \cdots, p_N$ plane.

The proof goes as follows. Let us denote the tangent plane by λ and the basis vectors defined by the phase space coordinate system $(x_1, \cdots, x_N, p_1, \cdots, p_N)$ by $\hat{x}_1, \cdots, \hat{p}_N$. Then each of the basis vectors $\hat{x}_1, \cdots, \hat{x}_k$ is contained in the projection of λ onto configuration space. That is, we can write

$$\hat{x}_i = l_i + \xi_i \tag{A1}$$

for each $i \leq k$, where l_i is in λ and ξ_i is in P. Now let $\xi_0 = \sum_i \alpha_i \hat{p}_i$ be an arbitrary vector in $\lambda_0 \equiv \lambda \cap P$. Using the fact that

$$[\hat{x}_i, \hat{p}_j] = \delta_{ij}, \tag{A2}$$

where $[\ ,\ ]$ denotes the symplectic form, we find that, for $i \leq k$,

$$\begin{aligned} \alpha_i &= [\hat{x}_i, \xi_0] \\ &= [l_i, \xi_0] + [\xi_i, \xi_0] \\ &= 0 + 0. \end{aligned} \tag{A3}$$

The product $[l_i, \xi_0]$ is zero because l_i and ξ_0 are both in the Lagrangian plane λ and $[\xi_i, \xi_0] = 0$ because ξ_i and ξ_0 are both in the Lagrangian plane P. Therefore we can conclude that ξ_0 is in the $p_{k+1}, \cdots, p_N$ plane, as required.

Because λ_0 is contained in the $p_{k+1}, \cdots, p_N$ plane, it follows from an argument of Arnol'd's[5,17] that $(x_1, \cdots, x_k)$ can be chosen as part of a good representation. We present the argument here for the sake of completeness.

Let us suppose that $\lambda_0 = \lambda \cap P$ is m-dimensional. Because it is m-dimensional it follows that λ_0 is tranverse in P to at least one $(N-m)$-dimensional coordinate plane τ, which is spanned by $N-m$ of the p-axes. Because λ_0 is contained in the plane spanned by the $p_{k+1}, \cdots, p_N$ axes we can further conclude that τ may be chosen so as to contain the $p_1, \cdots, p_k$ axes. Without loss of generality we can assume that τ is the plane spanned by the $p_1, \cdots, p_k, p_{k+1}, \cdots, p_{N-m}$ axes. We wish to show that a good representation is $x_1, \cdots, x_{N-m}, p_{N-m+1}, \cdots, p_N$. (Note that this representation includes $x_1, \cdots, x_k$.) We do this by showing that λ is transverse to the plane σ spanned by the $p_1, \cdots, p_{N-m}, x_{N-m+1}, \cdots, x_N$ axes *i.e.*, that $\lambda \cap \sigma = 0$. The following facts are straightforward consequences of the definitions:

$$\lambda_0 + \tau = P, \tag{A4(a)}$$

$$[\lambda, \lambda_0] = 0, \tag{A4(b)}$$

$$[\sigma, \tau] = 0, \tag{A4(c)}$$

where $\lambda_0 + \tau$ denotes the direct sum of λ_0 and τ. $A4(a)$ holds because τ is transverse to λ_0 in P, by definition, $A4(b)$ follows because λ_0 is contained in λ, which is Lagrangian, and finally $A4(c)$ holds because τ is contained in σ, which is also Lagrangian. All three of these together imply that

$$0 = [\lambda \cap \sigma, \lambda_0 + \tau] = [\lambda \cap \sigma, P]. \tag{A1.5}$$

Therefore $\lambda \cap \sigma$ is contained in the skew-orthogonal complement of P. However, because P is Lagrangian, its skew-orthogonal complement is just P itself. We can

therefore write,

$$\begin{aligned}\lambda \cap \sigma &= (\lambda \cap \sigma) \cap P \\ &= (\lambda \cap P) \cap \sigma \\ &= \lambda_0 \cap \sigma \\ &= 0\end{aligned}$$

It follows that λ is transverse to σ, so $x_1, \cdots, x_{N-m}, p_{N-m+1}, \cdots, p_N$ is a good representation.

Appendix B

In this appendix we describe two practical methods for determining σ that have been useful in numerical computations. The first method is useful for kinetic-plus-potential systems because it works even when the periodic orbits have cusps. The second method applies specifically to billiard systems and makes use of the fact that, for such systems, the surface of section mappings are easily computed analytically from the geometry of the periodic orbits. In each of these methods, σ is determined from the formula $\sigma = \mu + \nu$ rather than from the interpretation of σ as the Maslov index of the invariant manifolds.

Let us begin with a discussion of the determination of σ for kinetic-plus-potential systems. As discussed in Sec. 3 the surfaces of section and their mappings will often be ill-defined on of the periodic orbits of these systems. For a systematic treatment of the Maslov index in these systems it is therefore desirable to use a method which does not rely on the construction of the surfaces of section. To this end we will describe how to determine the Maslov index of an invariant Lagrangian manifold by propagating a frame of N vectors, tangent to the manifold, along a trajectory. This procedure can be applied to the Lagrangian manifold L of the energy-dependent Green's function, to determine μ in $\sigma = \mu + \nu$. By using this construction, μ is determined without reference to the surfaces of section. The remaining contribution, ν, is easily found from a reduction of the dynamics to a single surface of section, constructed at the initial/final point of the periodic orbit. Because it relies on the construction of just a single surface of section, this method should not be expected to fail for a kinetic-plus-potential system.

The first step in determining μ is to find N vectors that are tangent to the Lagrangian manifold at a reference point. For the energy-dependent Green's function the reference point is at the initial point, $\mathbf{x}'$, of the contributing trajectory. The N vectors we choose are the flow vector of the Hamiltonian X_H, which is tangent to L because L is invariant, and an additional $N-1$ vectors, $(e_1, \cdots, e_{N-1})$, which span the initial surface $\{ H = E, \mathbf{x} = \mathbf{x}' \}$. Assuming that $\dot{x}_N \neq 0$ we choose the vectors e_i to be such that their only non-zero components are $\Delta p_i = 1$ and $\Delta p_N = -\dot{x}_1/\dot{x}_N$. The component Δp_N is chosen so that an infinitesemal displacement along e_i conserves energy. These N vectors span the tangent plane to L at the initial point of the trajectory. We find a basis for the tangent plane to L at subsequent points on the trajectory by propagating $(e_1, \cdots, e_{N-1}, X_H)$ along it with the linearised dynamics. We denote the frame of vectors obtained in this way by $(e_1(t), \cdots, e_{N-1}(t), X_H(t))$. This frame of vectors completely determines μ.

Let us arrange the N vectors in the frame $(e_1(t), \cdots, e_{N-1}(t), X_H(t))$ so that they are the columns of a $2N \times N$ matrix T. Separating the $\mathbf{x}$ and $\mathbf{p}$ components, we can regard T as being made up of the $N \times N$ matrices U and V. That is we write

$$T = \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} u_1 & \dots & u_{N-1} & \dot{\mathbf{x}} \\ v_1 & \dots & v_{N-1} & \dot{\mathbf{p}} \end{pmatrix}, \qquad (C1)$$

where u_i and v_i are, respectively, the configuration space and momentum space components of e_i, and $X_H = (\dot{\mathbf{x}}, \dot{\mathbf{p}})$. The symmetric matrix R of Eq. (2.2.3), whose changes in signature determine the Maslov index, is obtained from T according to

$$R = UV^{-1}. \qquad (C2)$$

In writing this equation for R, we have used the $\mathbf{p}$ representation, which is a good representation provided V is invertible. We can see that Eq. (A3.2) holds by noting that an alternative basis for the Lagrangian plane is obtained by selecting the column vectors of the matrix $T' = TV^{-1}$. (The columns of T' are linear combinations of the vectors $(e_1(t), \cdots, e_{N-1}(t), X_H(t))$.) Noting that

$$T' = \begin{pmatrix} UV^{-1} \\ I \end{pmatrix}, \qquad (C3)$$

we can just read off the relationship $R = \partial \mathbf{x}/\partial \mathbf{p} = UV^{-1}$.

The caustics occur when U is singular. A null eigenvector of U specifies the components, in the basis $(e_1(t), \cdots, e_{N-1}(t), X_H(t))$, of a vector in the intersection of the Lagrangian plane with momentum space. For general Hamiltonians we must follow the eigenvalues of the matrix R in order to determine the contribution to the Maslov index from caustics. There is a significant simplification however, in the case that the Hamiltonian is of the type, kinetic plus potential, because for such systems it can be shown[5,10,11] that the Maslov index always increments at caustic crossings. The Maslov index over the whole trajectory can therefore be obtained simply by counting the number of places at which the condition $\det U = 0$ is satisfied. Finding and counting the zeros of $\det U$ is much easier than following the eigenvalues of R.

Having found μ for a periodic orbit, we next determine ν. The first step in determining ν is to locate the periodic orbit on some surface of section, which is formed by setting a configuration space coordinate to a constant value. Very often the periodic orbits are found in the first place by means of a search in such a surface of section, so this may be done already. Without loss of generality we can suppose that the surface of section is specified by $x_N = 0$. The surface of section must be chosen so that the periodic orbit crosses it transversely in configuration space, so we are at liberty to choose the $\mathbf{y}$ coordinates of Sec. 3 so that they coincide locally with the coordinates $(x_1, \cdots, x_{N-1})$ at the surface of section. The surface of section $x_N = 0$, with its coordinates $(x_1, \cdots, x_{N-1})$, then coincides with the surface of section $z =$ const., with its coordinates $\mathbf{y}$. We can therefore determine ν from the surface of section matrix M, constructed from the surface of section $x_N = 0$ using the coordinates $(x_1, \cdots, x_{N-1})$; it is the number of negative eigenvalues of the symmetric matrix $W = B^{-1}A + DB^{-1} - B^{-1} - \tilde{B}^{-1}$, where A, *etc*, are the block entries of M, as defined by Eq. (3.2).

Suppose now that one wanted to determine σ numerically for some list of periodic orbits. Then according to the calculations above we have the following algorithm. First one finds each periodic orbit in some surface of section of the form $x_N = 0$. Having done this, one propagates the N vectors $(e_1, \cdots, e_{N-1}, X_H)$ along the orbit, beginning at the surface of section. The initial values for the vectors $(e_1, \cdots, e_{N-1})$ are along the momentum axes of the surface of section. They are

propagated using the linearised equations of motion,

$$\dot{e}_i = JH''e_i, \tag{C4}$$

where H'' is the matrix of second derivatives of H, evaluated on the orbit, and J is the unit symplectic matrix. It is not necessary to integrate any differential equations explicitly for X_H since it is determined everywhere by Hamilton's equations. From the configuration space components of $e_i(t)$ and $X_H(t)$ one then constructs the matrices $U(t)$ along the orbit. The Maslov index μ is equal to the number of zeros of the function $\det U(t)$. The next step is to find the surface of section matrix M. To do this one propagates an additional $N-1$ vectors around the orbit, whose initial values are along the x-axes of the surface of section; together with e_i these vectors completely determine M. The index ν is then the number of negative eigenvalues of the matrix W, computed from M. Finally one computes $\sigma = \mu + \nu$.

By a slight modification of the procedure described above, according to which we determined the Maslov index μ of the energy-dependent Green's function, we can determine σ directly as the Maslov index of the invariant manifolds. The only difference is that we choose the vectors e_i, in the initial surface of section, to be say, the unstable eigenvectors of M, rather than choosing them to be along the momentum axes of the surface of section. With this choice for the initial vectors, the frame $(e_1, \cdots, e_{N-1}, X_H)$ spans the tangent plane of the unstable manifold along the orbit. For general Hamiltonians σ is determined by the changes in signature of the matrix $R = UV^{-1}$, constructed from this frame. For Hamiltonians that are of the form, kinetic plus potential, σ is simply the number of zeros of $\det U$ taken over one iteration of the orbit.

Alternatively, it can be shown[4,5] that σ is the winding number of the following closed curve in the complex plane,

$$z(t) = \det\Big\{(U - iV)(U + iV)^{-1}\Big\}, \tag{C5}$$

which in turn is equal to the winding number of the curve

$$z'(t) = \Big\{\det(U - iV)\Big\}^2. \tag{C6}$$

Though this second curve is not closed, it does return to its initial direction in the complex plane and therefore has a well-defined winding number. If one were to apply the full phase space method to σ for a general hamiltonian it would be advantageous to use Eq (C6), which requires us to keep track of a single complex number $z'(t)$, rather than the analysis based on R, which requires us to keep track of N eigenvalues. For kinetic plus potential systems however there is no practical advantage to be gained in using Eq. (C6).

The disadvantage of following the invariant manifolds as outlined above is that we need to follow the periodic orbit twice in order to determine σ. A preliminary iteration is needed to find the surface of section matrix M and once this is done, and the eigenvectors of M have been obtained, we need to iterate the orbit a second time in order to propagate the vectors e_i. On the other hand, using the method described above, in which μ and ν are determined seperately, the vectors e_i are found as part of the procedure for determining M and just one iteration of the periodic orbit is needed. However, if computing time is not a problem or if M is known already, the method of following the invariant manifolds may be easier to implement; it is certainly more pleasing aesthetically.

The methods discussed in this paper, employing surfaces of section constructed along the length of the periodic orbits, are well suited to billiard systems. This is because, given the lengths of the straight line segments and the angles of incidence at reflections, one can compute analytically the surface of section mappings for a given orbit.

In a billiard system the trajectories in configuration space consist of straight line segments connecting reflections from the boundary. In a two-dimensional billiard the straight line segments can be used as the basis for a rectangular coordinate system in the following way. We let y be the perpendicular distance from the trajectory and z be the distance along it; these coordinates define surfaces of section $\Sigma(z)$ specified by the condition $z = \text{const}$. We construct the linearised surface of section mappings M between these surfaces of section as follows. The mapping between two surfaces of section on the same straight line segment, separated by a

distance L, is the following free particle shear in the (y, p_y) coordinates,

$$M_{\text{trans}} = \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & L/p \\ 0 & 1 \end{pmatrix}, \tag{C7}$$

where $t = L/p$ is the time taken to go from one surface of section to the other with velocity p. The mapping that takes a surface of section that lies just before a reflection to one that lies just after it is

$$M_{\text{refl}} = \begin{pmatrix} -1 & 0 \\ 2p/\rho\cos\theta & -1 \end{pmatrix}, \tag{C8}$$

where ρ is the radius of curvature of the boundary at the point of reflection and θ is the angle of incidence of the trajectory there. The mapping between two arbitrary surfaces of section can now be built up from a sequence of translational segments, interspersed with reflections from the boundary a follows:

$$M = M_{\text{trans}} M_{\text{refl}} \cdots M_{\text{refl}} M_{\text{trans}}. \tag{C9}$$

In this way we can analytically construct the surface of section mappings from a knowledge of the basic geometry of the orbit.

Let us now consider the Maslov index μ of the energy-dependent Green's function. Unlike the case of smooth systems, the Maslov index in billiards is not determined solely by caustics; μ must be incremented by 2 at every reflection from the boundary. These contributions from the boundary are such that the Green's function satisfy the boundary condition that it vanish there. The increment of μ by two gives the corresponding two branches of the Green's function a phase difference of π at the boundary, so that they cancel there making the Green's function vanish. In addition to the contributions from reflections, one also has contributions from regular internal caustics. These are determined by the vanishing of the b component of the surface of section matrix M, as described in Sec. 3. Because b varies linearly with distance along the straight line segments, there can be at most one caustic between every reflection. One therefore needs only to check whether b has changed sign on going from one reflection to the next. An added simplification is that, because the dynamics is like that of a free particle in the interior of the billiard, the

Maslov index always increments at caustics, so μ is obtained from a simple count of the zeros of b.

It is sometimes useful to think of the problem of finding caustics in terms of geometrical optics. The reflections from the boundary are like reflections from spherical mirrors that have an effective focal length of $\frac{1}{2}\rho\cos\theta$. The caustics are then the images formed when an object is placed at the initial point of the orbit; the caustics are a result of the focussing that occurs after trajectories reflect from the boundary. In this picture for example it is obvious that a boundary that is made up entirely of dispersing, concave inward, components will not give rise to internal caustics. For such systems, μ is just twice the number of reflections. A system whose boundary has focussing components, such as the stadium,[13,14] will have internal caustics however, and these need to be taken into account for a full evaluation of the Maslov index.

Finally, the index ν is computed from the surface of section matrix taken from a full iteration of the periodic orbit as described in Sec. 4. The trace formula index is then $\sigma = \mu + \nu$.

Just as discussed for the previous case of kinetic-plus-potential Hamiltonians, one can apply similar methods to obtain the index σ from the evolution of the invariant manifolds. If an eigenvector of M is propagated around the orbit, the index σ is equal to the number of times the eigenvector passes through the p_y-axis plus twice the number of reflections from the boundary. Once again however, this method has the disadvantage that it necessitates following the dynamics around the periodic orbit twice; once to find M and a second time to propagate the invariant manifolds.

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References

1. M. C. Gutzwiller, J. Math. Phys. **8**, 1979 (1967); **10**, 1004 (1969); **11**, 1791 (1970); **12**, 343 (1971).
2. R. Balian and C. Bloch, Ann. Phys. (N.Y.) **60**, 401 (1970); **63**, 592 (1971); **69**, 76 (1972); **85**, 514 (1974).
3. J. M. Robbins, To be published
4. J. M. Robbins, Ph.D. Thesis, University of California. Berkeley (1989).
5. V. I. Arnol'd, Functional Anal. Appl. **1**, 1 (1967).
6. V. P. Maslov, *Théorie des Perturbations et Méthodes Asymptotiques* (Dunod, Paris, 1972).
7. V. P. Maslov and M. V. Fedoriuk, *Semi-Classical Approximation in Quantum Mechanics* (Reidel, Boston, 1981).
8. J. B. Delos, Adv. Chem. Phys. **65**, 161 (1965).
9. I. C. Percival, Adv. Chem. Phys. **36**, 1 (1977).
10. S. Levit, K. Möhring, U. Smilansky and T. Dreyfus, Ann. Phys. **114**, 223 (1978).
11. K. Möhring, S. Levit and U. Smilansky, Ann. Phys. **127**, 198 (1980).
12. R. G. Littlejohn, Submitted to J. Math. Phys.
13. S. W. McDonald, Lawrence Berkeley Laboratory Report No. LBL-14837, 1983 (unpublished).
14. S. W. McDonald and A. N. Kaufman, Phys. Rev. Lett. **42**, 1189 (1979).
15. E. B. Bogomolny, Physica D, **31**, 169 (1988).
16. J. M. Souriau, C. Rendus Acad. Sci. **276**, 1025 (1973).
17. V. I. Arnol'd, *Mathematical Methods of Classical Mechanics* (Springer, New York, 1978).

Figure Captions

Fig.1 The singular projection of a Lagrangian manifold onto configuration space as the two branches $b = 1$ and $b = 2$ coalesce at a caustic.

Fig.2 Shown here for the case of two degrees of freedom, the Lagrangian manifold L is swept out by the iniital surface $\{\mathbf{x} = \mathbf{x}'\}$ in the three-dimensional energy shell $\{H = E\}$.

Fig.3 Illustrated in the case of two degrees of freedom are, (a) a typical caustic crossing, (b) a degenerate caustic crossing in which the trajectory comes to rest and forms a cusp in configuration space.

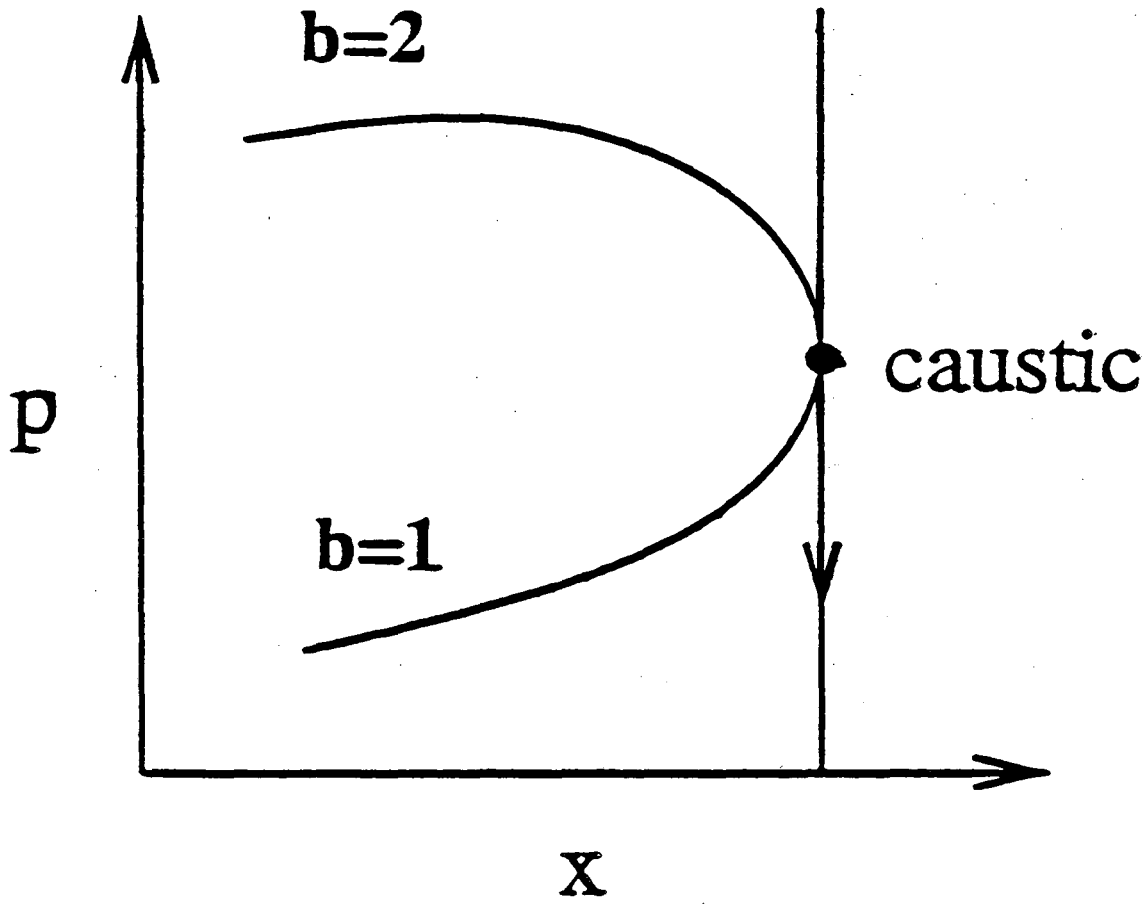
Fig.4 The mapping $F(z, z')$ carries the surface of section $\Sigma(z')$ into the surface of section $\Sigma(z)$ using the flow in a neighbourhood of the orbit.

Fig.5 The Lagrangian manifold L intersects a surface of section along the tangent plane λ at the periodic orbit.

Fig.6 In (a) a starting point on the diamond periodic orbit of the stadium billiard is chosen for which there is just one caustic. A slightly different starting point of the same orbit in (b) gives two caustics.

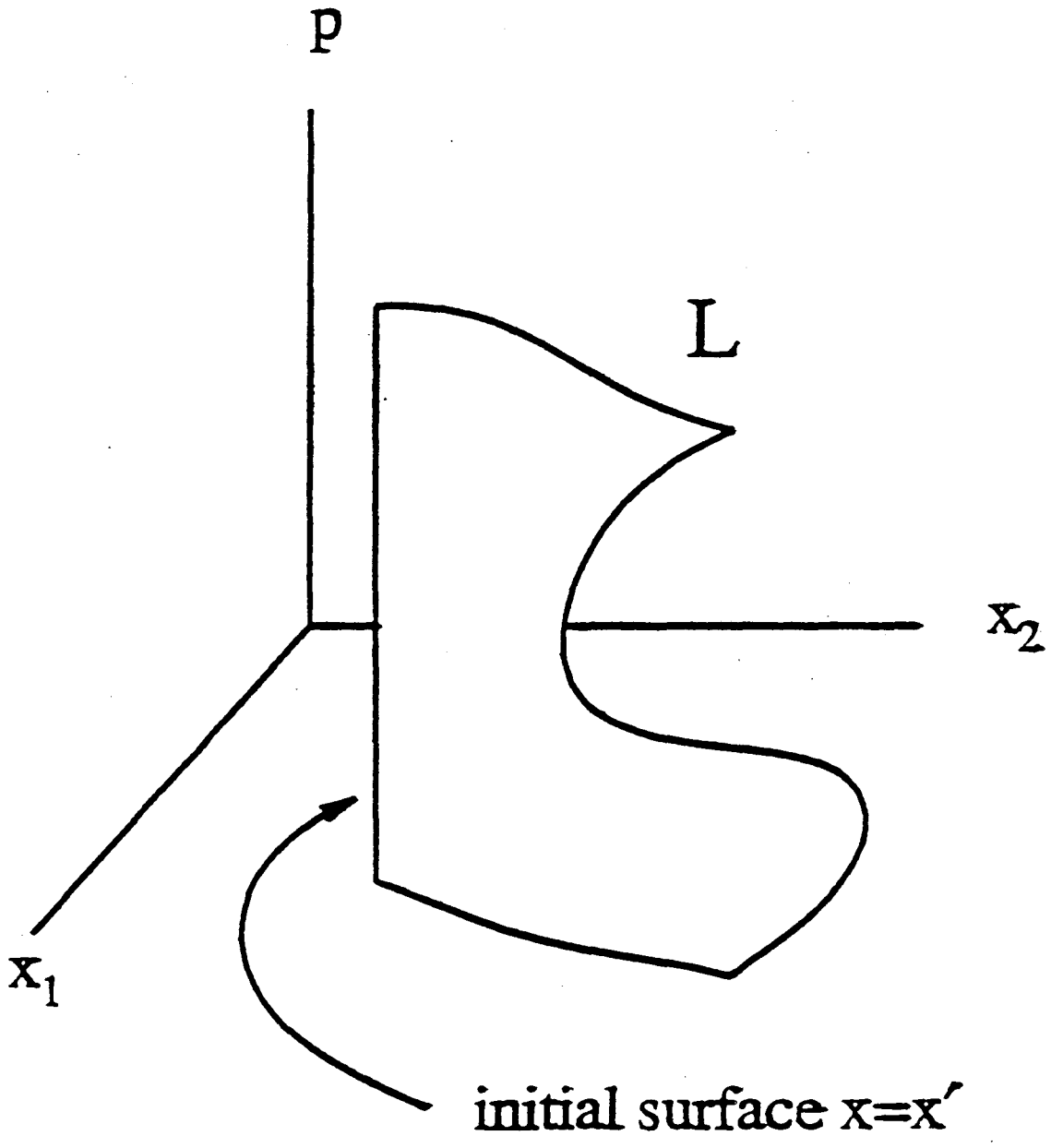
Fig.7 The final position of the line λ is determined by the hyperbolic structure of the surface of section mapping near the periodic orbit.

Fig.8 The division of the surface of section into the sectors H, I, J and K by the stable and unstable manifolds is illustrated in (a). The dependence of ν on the final position of λ within the sectors H and J is shown in (b).



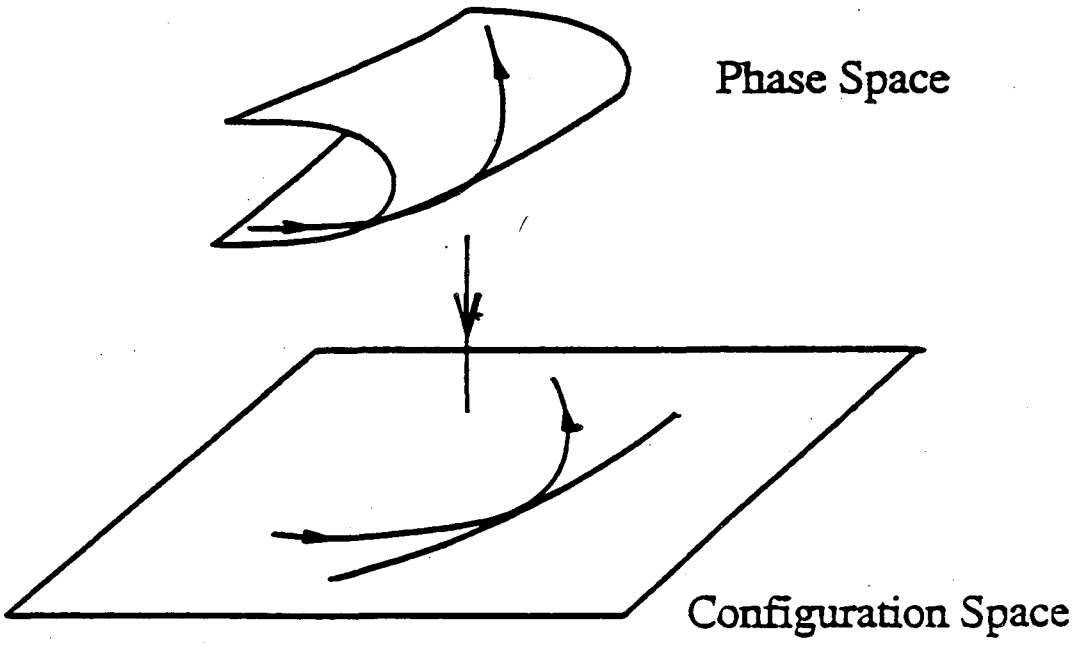
XBL 905-1929

Fig. 1



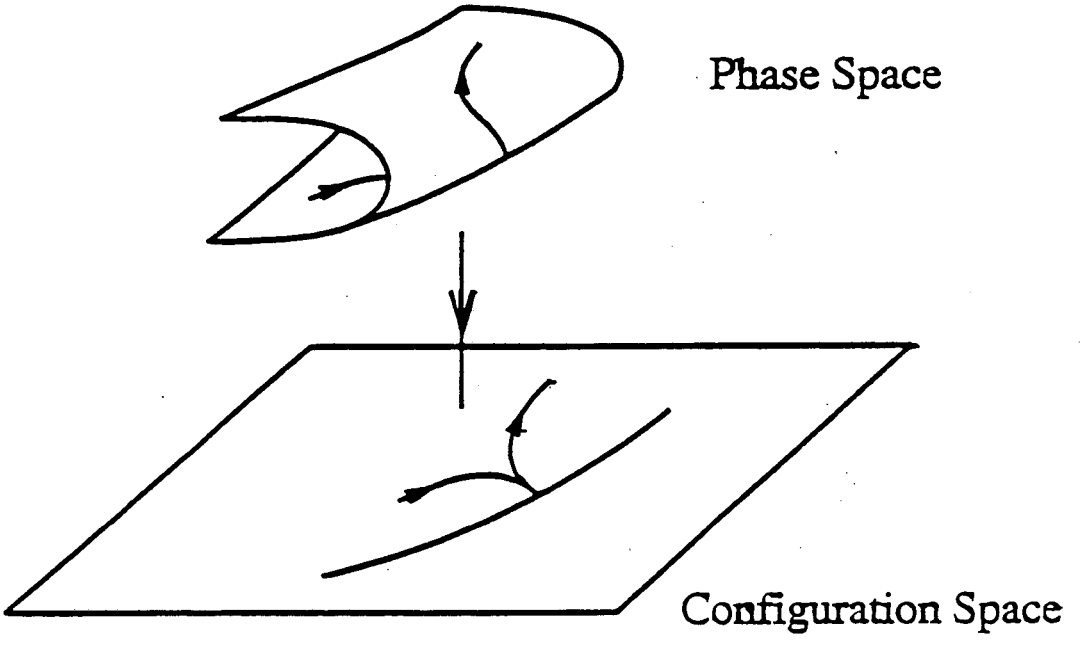
XBL 905-1930

Fig. 2



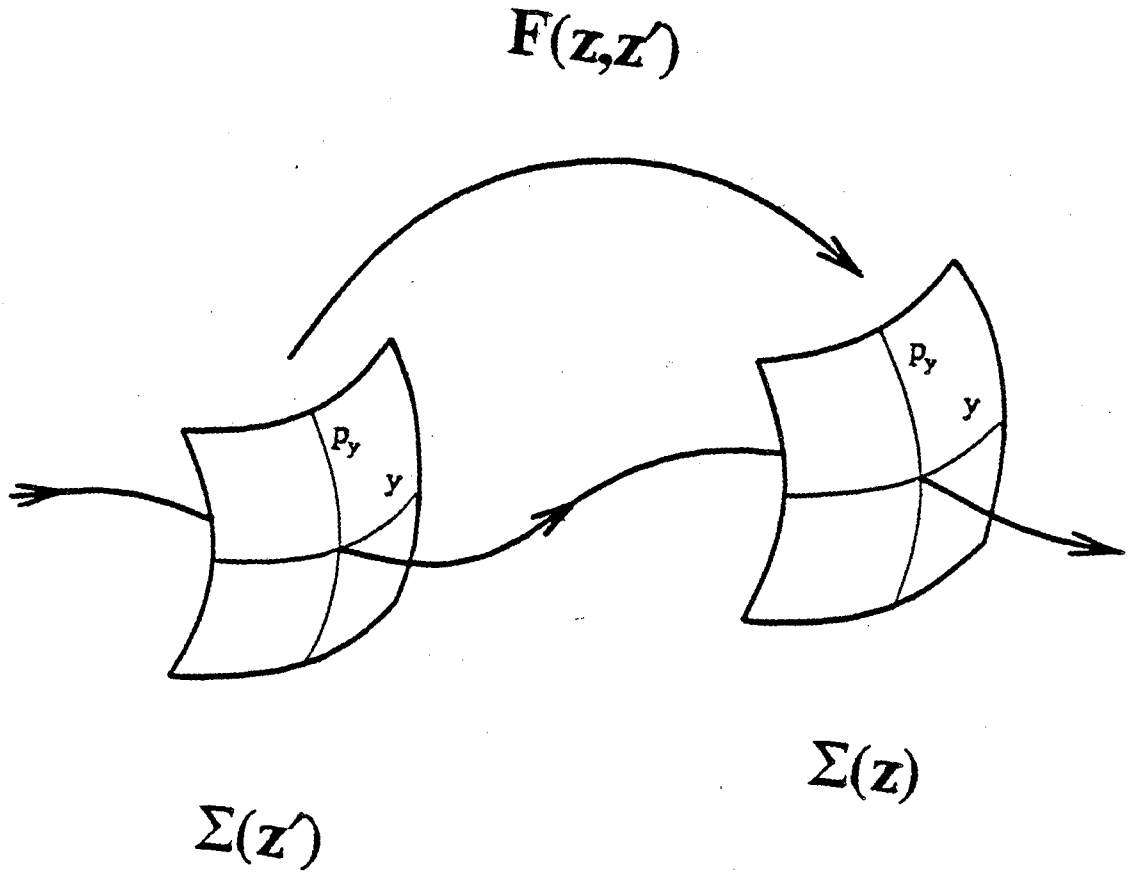
XBL 905-1931

Fig. 3a



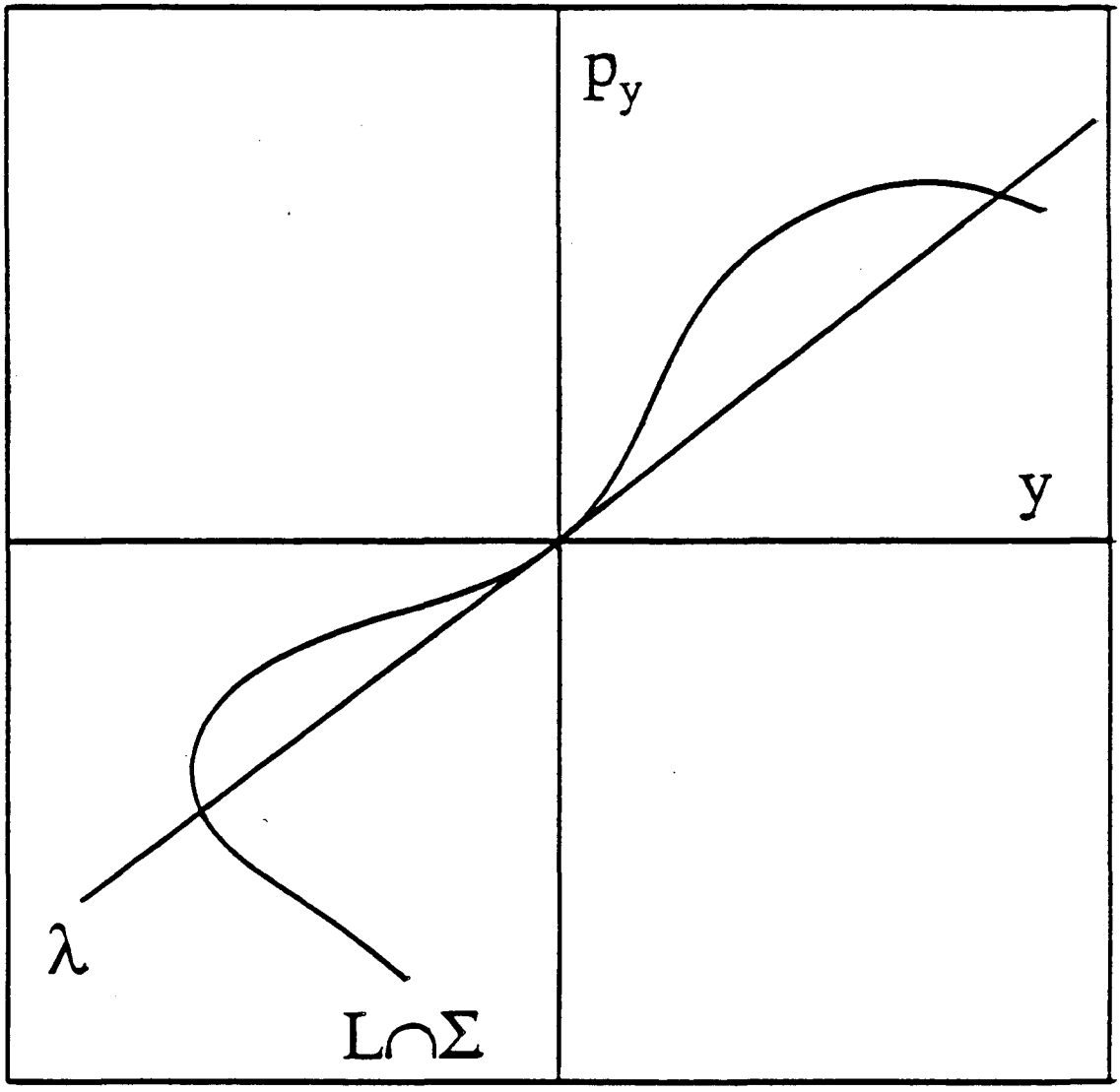
XBL 905-1932

Fig. 3b



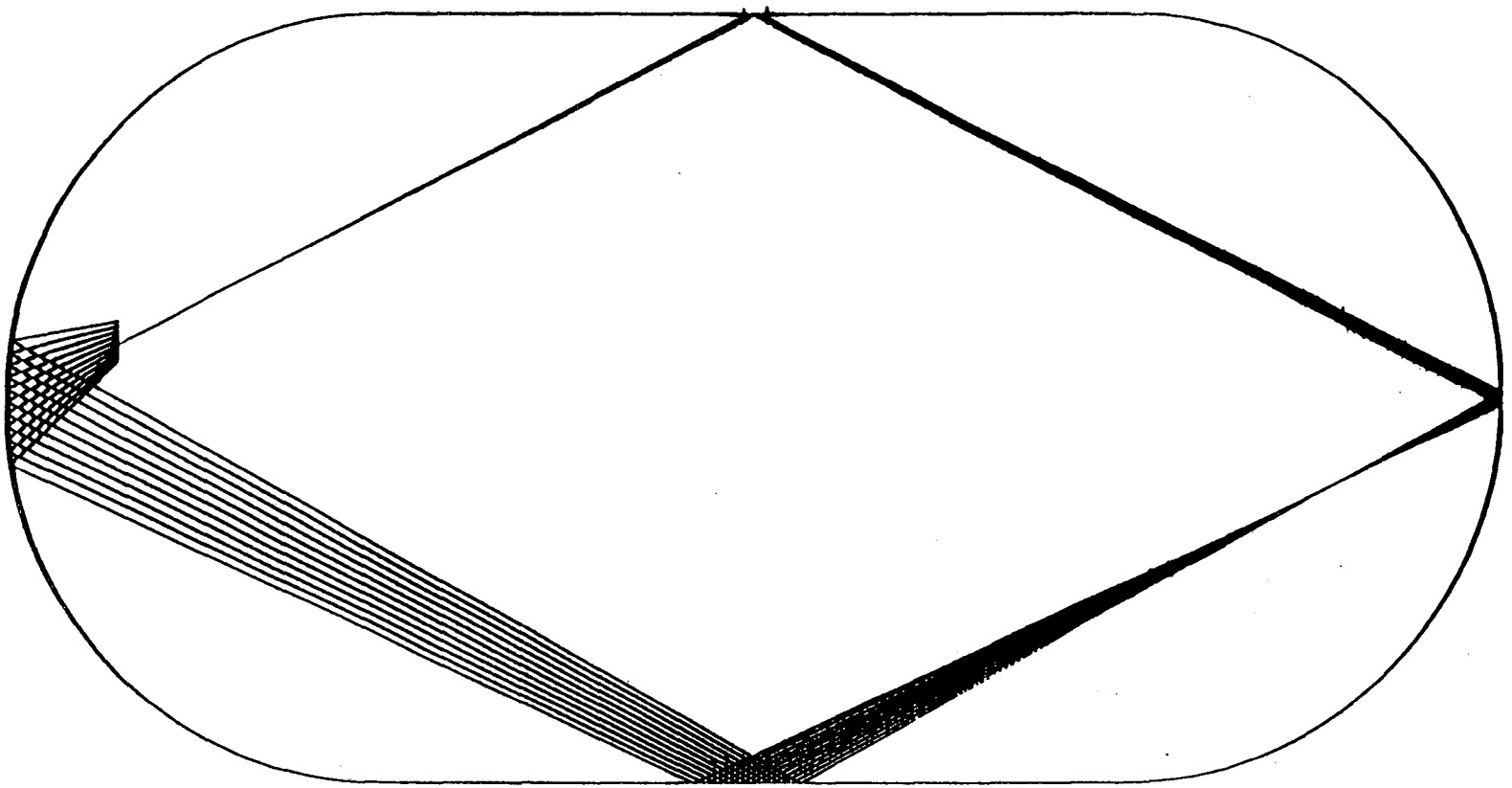
XBL 905-1933

Fig. 4



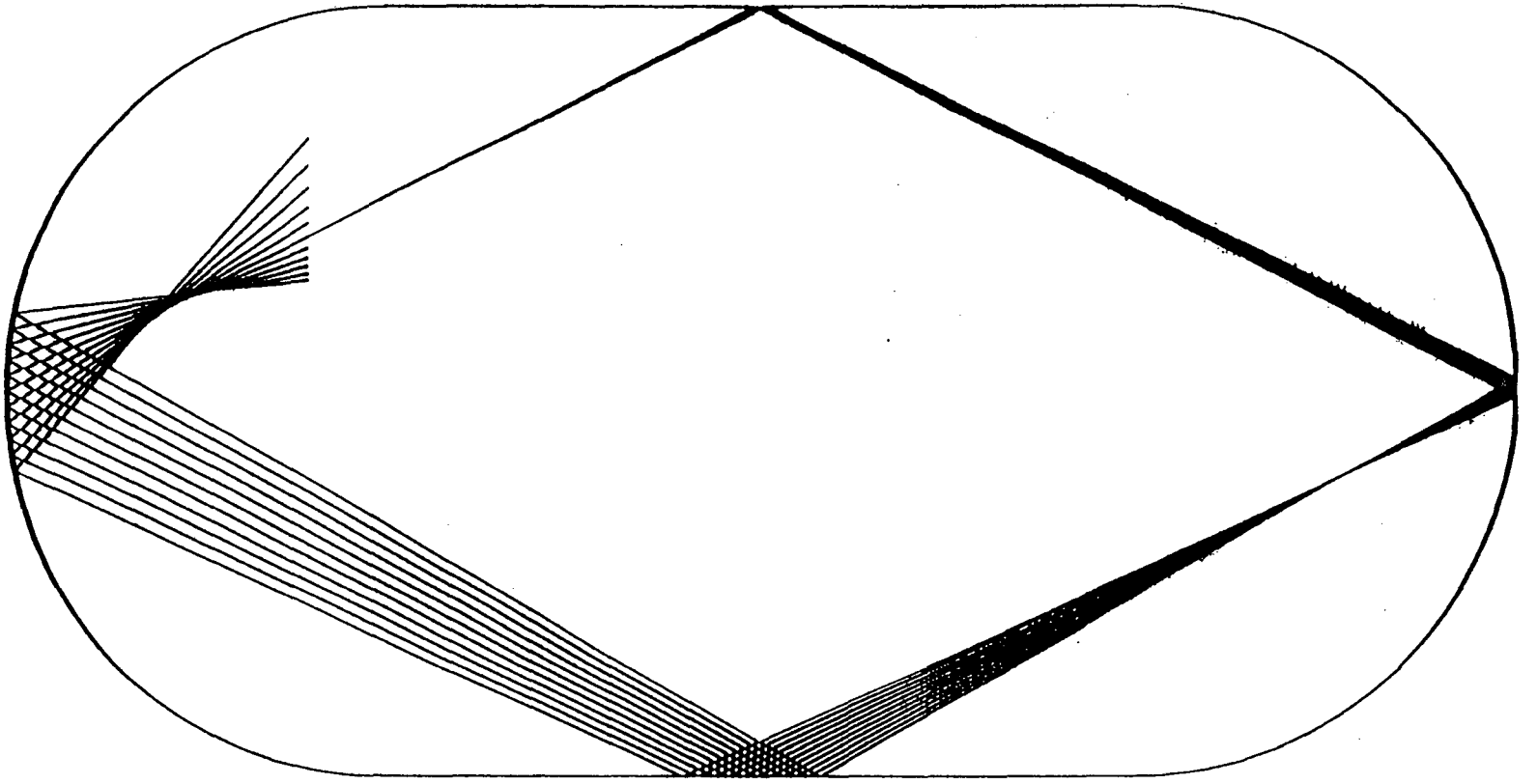
XBL 905-1934

Fig. 5



XBL 905-1935

Fig. 6a



XBL 905-1936

Fig. 6b

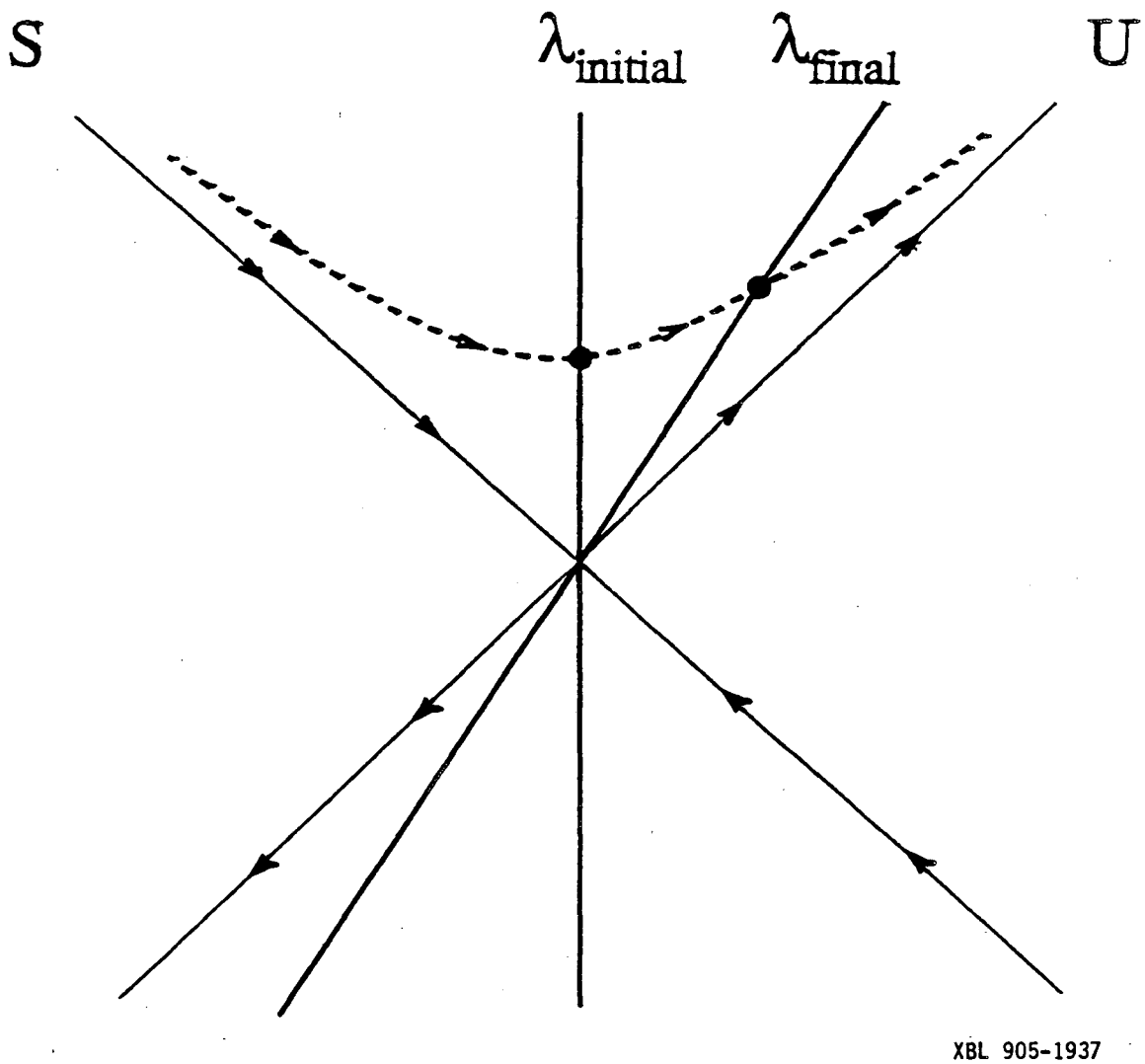
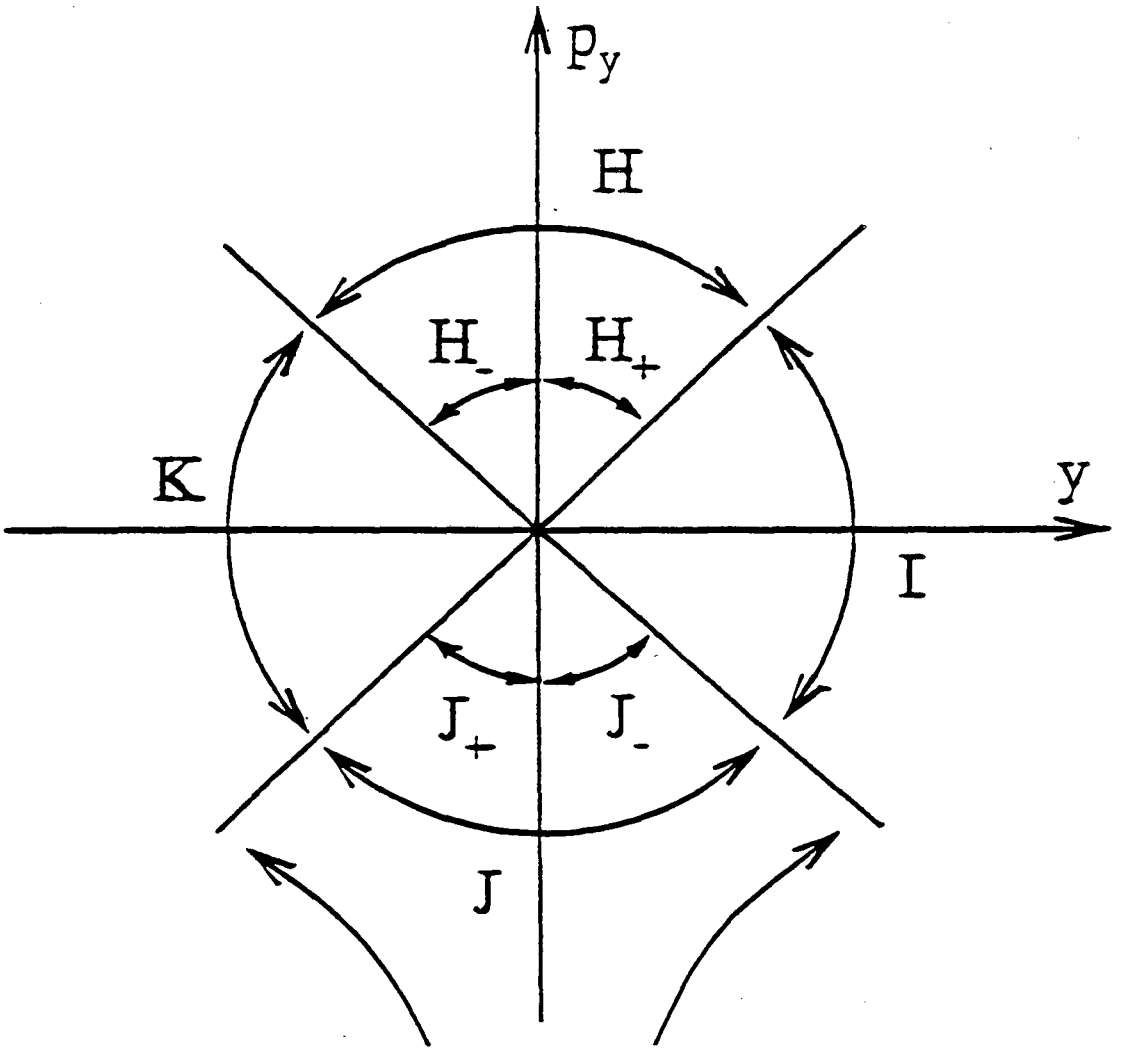


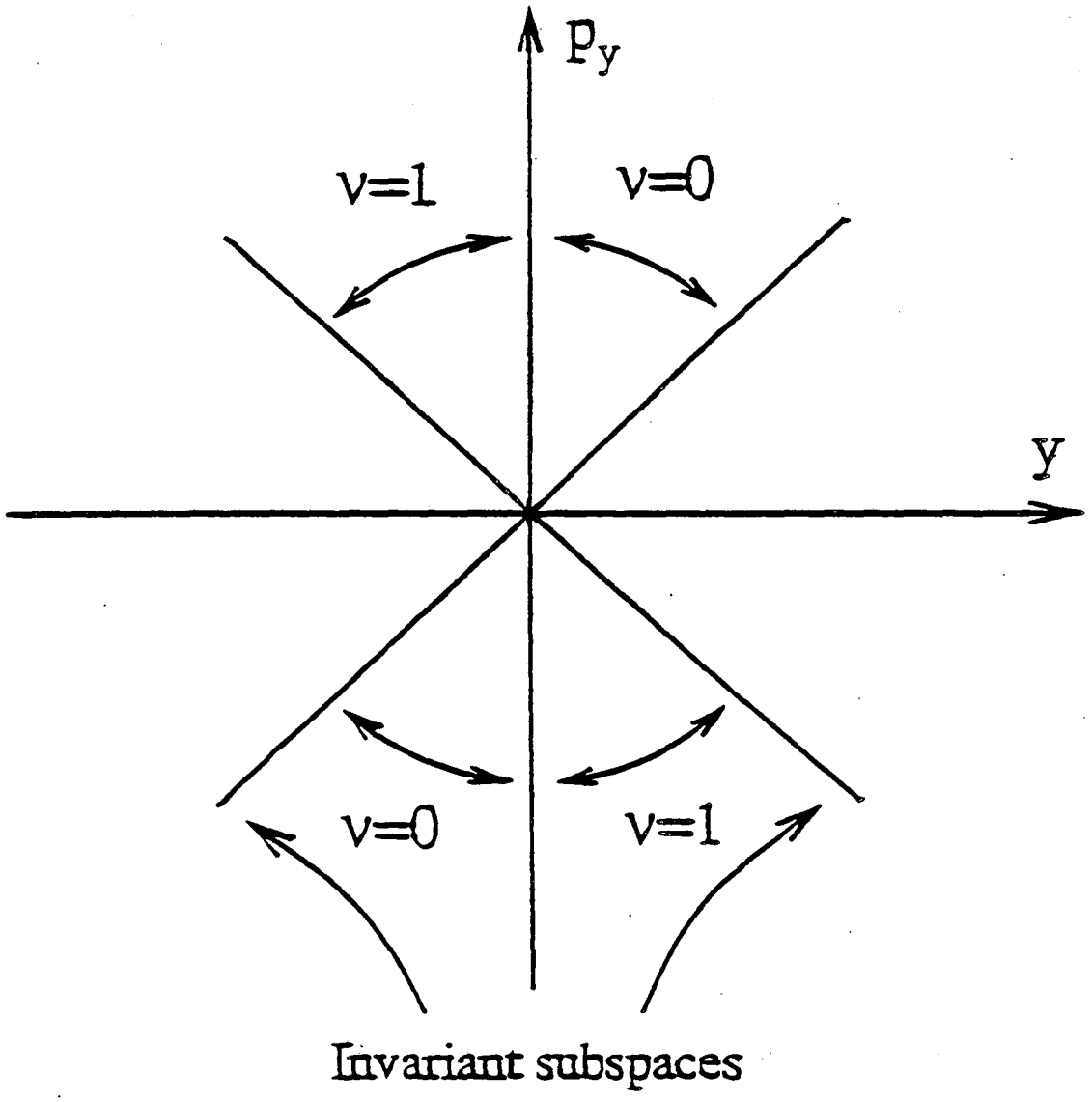
Fig. 7



Invariant subspaces

XBL 905-1938

Fig. 8a



XBL 905-1939

Fig. 8b

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