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# ARTICLES

## Semiclassical trace formulas in the presence of continuous symmetries

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We derive generalizations of the semiclassical trace formula of Gutzwiller [J. Math. Phys. **12**, 343 (1971)] and Balian and Bloch [Ann. Phys. **69**, 76 (1972)] that are valid for systems exhibiting continuous symmetries. In particular, we consider symmetries for which the associated set of conserved quantities Poisson-commute. For these systems, the periodic orbits of a given energy occur in continuous families and the usual trace formula, which is valid only when the periodic orbits of a given energy are isolated, does not apply. In the trace formulas we derive, the density of states is determined by a sum over continuous families of periodic orbits rather than a sum over individual periodic orbits. Like Gutzwiller's formula for isolated orbits, the sum involves intrinsic, canonically invariant properties of the periodic orbits. We illustrate the theory with two important special cases: axial symmetry and integrable systems.

### I. INTRODUCTION

Semiclassical trace formulas, as developed by Gutzwiller [1], and Balian and Bloch [2], are the only means presently available of using classical mechanics to investigate the spectra of quantum-mechanical systems when the classical dynamics is nonintegrable. These formulas express approximately the density of states $\rho(E)$ of a quantum-mechanical Hamiltonian as a sum over the periodic orbits of the corresponding classical Hamiltonian. For example, the Gutzwiller trace formula approximates the oscillating part of the density of states as the following discrete sum over periodic orbits:

$$\rho(E)\approx\frac{1}{\pi\hbar}\sum_{\substack{\text{periodic}\\ \text{orbits}}}\frac{T_0}{|\det(M-I)|^{1/2}}\cos\left[\frac{1}{\hbar}S-\sigma\frac{\pi}{2}\right]. \tag{1.1}$$

Here $T_0$ is the period of the primitive periodic orbit and the stability matrix $M$ is the linearization of a surface of section mapping at the periodic orbit. $S$ is the action of the orbit and $\sigma$ is the Maslov index of the periodic orbit's stable and unstable manifolds [3–4].

Equation (1.1) has been applied with considerable success to systems whose classical dynamics is completely chaotic [5–9], in which case the periodic orbits of a given energy are isolated in phase space and the totality of such periodic orbits forms a discrete set. More generally, one could, in principle, use Eq. (1.1) for mixed systems, where island chains coexist with regions of stochasticity in phase space, to find that part of the spectrum corresponding to the stochastic regions of phase space [while torus (or EBK) quantization could be used on the island chains]. Many important physical systems, however, fall into neither of these categories, and in such a way that Eq. (1.1) cannot be applied to them—these are systems with continuous symmetry.

The discrete sum of Eq. (1.1) does not apply when periodic orbits occur in continuous families, as is the case when a continuous symmetry is present. While such situations are exceptional in a mathematical sense, they are relatively common in physical applications. For example, problems with three-dimensional rotational symmetry occur quite often, as do problems with just axial symmetry. Trace formulas for rotationally symmetric systems might have important applications to small atomic systems such as the helium atom, which are nonintegrable but have few enough degrees of freedom that they might be amenable to a periodic orbit analysis. In addition, the shell structure of nuclei has been interpreted in terms of fluctuations in the density of states due to periodic orbits of nucleons in the spherically symmetric mean field of the nucleus [2,11–13]. Of special interest in this paper will be systems with axial symmetry, of which the hydrogen atom in a strong magnetic field is an example that has received much attention recently [6,7]. It would be of considerable interest to be able to apply trace formulas like Eq. (1.1) in a systematic and coherent way to the systems outlined above and to other systems with symmetry. It is to this issue that we will address ourselves in this paper.

In this paper we will derive generalizations of Eq. (1.1) that apply to systems for which any two first integrals Poisson-commute—these first integrals are necessarily associated with an Abelian symmetry through Noether's

 

theorem. These systems include, as special cases, systems for which there is a single first integral in addition to the Hamiltonian—such as axial symmetry, for example—and integrable systems. We will treat the more general case of non-Abelian symmetry in a subsequent paper. While trace formulas have been derived for systems with nonisolated periodic orbits before, such formulas do not have the power and elegance of the trace formula for isolated orbits, as developed by Gutzwiller—unlike Gutzwiller's formula, these results have been applicable only to very specific types of systems and/or have had a complicated dependence on the classical dynamics.

Balian and Bloch [2] developed trace formulas for billiard systems with arbitrary degrees of symmetry. However, their results depend in a somewhat complicated way on the classical dynamics and would be difficult to apply directly to a concrete example. (An exception is the important example of a spherical cavity, for which they obtain detailed results.) Strutinski and Magner [11] have given an extensive analysis of the effects of symmetry on systems with a smooth potential (with applications to nuclear shell structure), but find explicit results only for systems of three degrees of freedom. Berry and Tabor [14] have derived a trace formula for integrable systems which has an intrinsic dependence on the classical dynamics (through action-angle variables), but their results do not apply to nonintegrable systems with symmetry. As well as the calculations above for direct analogs of the Gutzwiller trace formula, closely related formulas relating the spectra of certain classes of operators to classical periodic orbits have been derived by Chazarain [15] and Duistermaat and Guillemin [16]. They compute the trace of the propagator (rather than of the energy-dependent Green's function) for systems for which the classical Hamiltonian is homogeneous in momentum—for example, free-particle motion on a Riemannian manifold—and give explicit consideration to cases in which periodic orbits occur in continuous families. Duistermaat and Guillemin, in particular, derive results which are remarkably like Gutzwiller's, but they are valid only for a restricted class of systems.

In this paper, we will derive direct generalizations of Eq. (1.1) that are valid under quite general assumptions and have a relatively simple dependence on the classical mechanics. The only assumption is that any degeneracy of periodic orbits is due to the presence of a phase-space symmetry, which we assume to be Abelian in this paper. Using this symmetry, we compute trace formulas that depend on simple, intrinsic properties of the periodic orbits that are easily computed in practice, such as actions, periods, and surface of section mappings.

Consider the case of a three-degree-of-freedom system with axial symmetry, like the example of a hydrogen atom in a strong magnetic field, which we use to illustrate our results in Sec. IV. The usual way to treat this system is to use cylindrical polar coordinates $(\rho,\theta,z)$ on configuration space and to ignore the $\theta$ coordinate. By applying Eq. (1.1) to this reduced system, one obtains the density of states corresponding to a given magnetic quantum number $m$, where $m$ depends on the value of the momentum $p_\theta$ that is chosen for the reduced system, through $p_\theta = m\hbar$. Past applications have usually been applied to the case $m=0$ [6,7]. While this works quite well for the reduced density of states, there is no analogous procedure for the full density of states, for which it is important to use full phase-space dynamics. For example, orbits that are periodic in the reduced system will not always be periodic in the full phase space because they will, in general, not close in the $\theta$ coordinate.

The trace formula that we derive for such a system is a sum over orbits that are truly periodic and looks much like Eq. (1.1) [see Eq. (3.14)]. The surface of section matrix $M$ is replaced by a surface of section matrix for the reduced dynamics. The period of the primitive orbit $T_0$, which measures the length of the periodic orbit in terms of a time coordinate $t$, is replaced by a measure of the area of the two-dimensional manifold of periodic orbits in terms of the coordinates $(t,\theta)$, where $\theta$ is an angle of rotation about the symmetry axis. This is typically just $2\pi T_0$. In addition, there is another factor that has no analog in Eq. (1.1). This factor measures the amount by which periodic orbits of the reduced system that are close to the periodic orbit in question fail to close in the angular coordinate. It is explained in more detail in the main text. Notice that these quantities are no more difficult to calculate for axially symmetric systems than the various contributions to Eq. (1.1) would be for systems without symmetry.

A second special case of the systems that we consider in this paper is that of integrable systems. We illustrate this situation in some detail in Sec. IV. In this case, the periodic orbits correspond precisely to rational tori, and Eq. (1.1) is replaced by a sum over these tori. We specialize our results to these systems by writing them entirely in terms of action-angle variables. In doing so, we quite quickly arrive at results that are equivalent to those of Berry and Tabor [14], who derived an analog of Eq. (1.1) in two ways. In the first they used the Poisson sum formula to reexpress the torus quantization conditions in terms of a sum over rational tori. In the second, which is more like the methods used by us and by Gutzwiller, they used an angle-variable representation of the Green's function to evaluate its trace.

Before starting the calculations we give a brief outline of the structure of the paper. In Sec. II we begin the calculation of the density of states under the assumption that periodic orbits occur in continuous families. The calculations in this section are quite general and make no assumptions about symmetry. In Sec. III we specialize to the case that there are constants of motion in involution and use the resultant symmetry to find explicit results for the calculations of Sec. III. In Sec. IV we illustrate the results with the two special cases: axial symmetry and integrable systems.

## II. GENERAL THEORY

In this section, while making no explicit assumptions about the nature of periodic orbit families, we begin to compute a trace formula analogous to Eq. (1.1). We follow essentially the method of Gutzwiller [1], except modified to take into account the possibility that periodic

orbits occur in families. The result we obtain by the end of this section involves a nontrivial integral over each periodic orbit family and is therefore not directly useful in practical situations. However, it will provide a springboard for the calculations of later sections, where we make use of the symmetry properties of the system in question to compute the integrals.

Rather than dealing directly with the density of states $\rho(E)$, we find it convenient to work instead with the trace of the resolvant $1/E-H$,

$$g(E)\equiv \mathrm{Tr}\frac{1}{E-H}=\sum_n \frac{1}{E-E_n} , \tag{2.1}$$

where $E_n$ are the energy levels of the Hamiltonian $H$. This trace is related to the density of states through

$$\rho(E)=-\frac{1}{\pi}\,\mathrm{Im}\,g(E+i\epsilon) \tag{2.2}$$

for small positive $\epsilon$. If $\epsilon$ is allowed to be finite in Eq. (2.2) the result is a density of states that is averaged over an energy interval of width $\epsilon$, whereas in the limit $\epsilon\to 0$ the exact density of states is recovered [2]. In calculations such as ours it has often been assumed that $\epsilon$ is small but finite, because this has the desirable effect on the semiclassical approximations we use of eliminating contributions from long-term dynamics, where the approximations break down. It has the undesirable effect, however, of forcing us to consider dynamics for complex energies, a situation which is difficult to deal with. For this reason we will largely ignore the issue of $\epsilon$ being nonzero, assuming either that $\epsilon$ is small enough that it does not affect the classical dynamics or that $\epsilon=0$ and some other truncation procedure is in effect to eliminate the consequences of long-term dynamics.

We will use a mixed-representation Green's function to compute the trace in Eq. (2.1):

$$g(E)=\frac{1}{(2\pi\hbar)^{n/2}}\int dx'\int d\mathbf{p}\,\exp(i\mathbf{p}\cdot\mathbf{x}'/\hbar)G(\mathbf{p},\mathbf{x}',E) , \tag{2.3}$$

where

$$G(\mathbf{p},\mathbf{x}',E)\equiv\left\langle \mathbf{p}\left|\frac{1}{E-H}\right|\mathbf{x}'\right\rangle . \tag{2.4}$$

The basis of the calculation is the following semiclassical approximation for $G(\mathbf{p},\mathbf{x}',E)$ in terms of classical trajectories [1]:

$$G(\mathbf{p},\mathbf{x}',E)\approx\frac{1}{i\hbar}\frac{e^{i\nu\pi/4}}{(2\pi\hbar)^{(n-1)/2}}\sum D(\mathbf{p},\mathbf{x}',E)\exp\left[\frac{i}{\hbar}T(\mathbf{p},\mathbf{x}',E)-i\mu\pi/2\right] , \tag{2.5}$$

where the sum is taken over the classical trajectories of energy $E$ that start at position $\mathbf{x}'$ and end with momentum $\mathbf{p}$ in positive time. The integer $n$ is the number of degrees of freedom and the phase $T(\mathbf{p},\mathbf{x}',E)$ is the action,

$$T(\mathbf{p},\mathbf{x}',E)=-\mathbf{p}'\cdot\mathbf{x}'-\int_{\mathbf{x}'}^{\mathbf{p}}\mathbf{x}\cdot d\mathbf{p} . \tag{2.6}$$

The Maslov index $\mu$ is initially 0 and is incremented or decremented at subsequent momentum-space caustics according to the usual rules [3,4]. In addition, there is an extra phase contribution determined by the integer $\nu\equiv-\mathrm{sgn}(\partial E/\partial t)_{\mathbf{x}',\mathbf{p}'}$ to be evaluated near $t=0$. Finally, the amplitude $D(\mathbf{p},\mathbf{x}',E)$ can be written as a Jacobian,

$$D(\mathbf{p},\mathbf{x}',E)=\left|\left[\frac{\partial(\mathbf{p}',t)}{\partial(\mathbf{p},E)}\right]_{\mathbf{x}'}\right|^{1/2} , \tag{2.7}$$

where the subscript $\mathbf{x}'$ indicates that derivatives are taken while $\mathbf{x}'$ is held fixed. Here, and in the future, quantities related to the initial point of a trajectory are primed and quantities related to the final point of a trajectory are unprimed.

This approximation is derived in a straightforward way from the Van Vleck approximation for the mixed-representation propagator $K(\mathbf{p},\mathbf{x}',t)$, in which $K(\mathbf{p},\mathbf{x}',t)$ is expressed approximately as a sum over trajectories from $\mathbf{x}'$ to $\mathbf{p}$ of a given time $t$, much like Eq. (2.5) itself. The propagator $K(\mathbf{p},\mathbf{x}',t)$ is related to the Green's function $G(\mathbf{p},\mathbf{x}',E)$ through a Laplace transform in time, and on computing this transformation by means of the stationary phase approximation, one obtains Eq. (2.5).

Let us now begin to compute the trace. Inserting approximation (2.5) into Eq. (2.3), we find

$$g(E)\approx\frac{1}{i\hbar}\frac{1}{(2\pi\hbar)^{n-1/2}}\int d\bar{\mathbf{z}}\sum D(\mathbf{p},\mathbf{x}',E)\exp\left[\frac{i}{\hbar}S(\mathbf{p},\mathbf{x}',E)-i\mu\pi/2+i\nu\pi/4\right] , \tag{2.8}$$

where $\bar{\mathbf{z}}=(\mathbf{x}',\mathbf{p})$ and $S(\mathbf{p},\mathbf{x}',E)=T(\mathbf{p},\mathbf{x}',E)+\mathbf{p}\cdot\mathbf{x}'$. We will use the stationary phase approximation to compute the integral over $\bar{\mathbf{z}}$. Using the generating function conditions on $T(\mathbf{p},\mathbf{x}',E)$, the stationary phase conditions are

$$0=\frac{\partial S(\mathbf{p},\mathbf{x}',E)}{\partial\mathbf{x}'}=-\mathbf{p}'+\mathbf{p} , \tag{2.9a}$$

$$0=\frac{\partial S(\mathbf{p},\mathbf{x}',E)}{\partial\mathbf{p}}-\mathbf{x}+\mathbf{x}' . \tag{2.9b}$$

There are two distinct kinds of trajectory for which this stationary phase condition holds. The first is that of the so-called zero-length orbits, which are limiting cases of short-time orbits connecting $(\mathbf{x}',\mathbf{p}')$ to some nearby

$(\mathbf{x},\mathbf{p})$. Equation (2.5) does not properly represent these orbits—the end-point corrections from the $t=0$ limit of the Laplace transform relating $G(\mathbf{p},\mathbf{x}',E)$ to $K(\mathbf{p},\mathbf{x}',t)$ are important for such orbits, but are not included in Eq. (2.5). However, using improved approximations it is possible to compute the contribution of zero-length orbits to the density of states. This calculation has been performed by Berry and Mount [17] and is not affected by the presence of a continuous symmetry, so their calculations apply equally well to the systems we want to consider. The result is the Thomas-Fermi density of states $\rho_{\rm TF}(E)$,

$$\rho_{\rm TF}(E)=\frac{1}{(2\pi\hbar)^n}\int d\mathbf{x}\,d\mathbf{p}\,\delta(E-H(\mathbf{x},\mathbf{p}))\ , \tag{2.10}$$

which represents an average of $\rho(E)$ over an energy scale that is large compared with $O(\hbar)$.

The second case of the stationary phase condition occurs when the trajectory connecting $\mathbf{x}'$ to $\mathbf{p}$ is a periodic orbit, and the contribution from these orbits is profoundly affected by the presence of continuous symmetries. The contribution from periodic orbits to the density of states, $\rho_{\rm osc}(E)$ say, represents fluctuations of $\rho(E)$ away from the mean behavior of Eq. (2.10) with an energy scale $\Delta E\sim O(\hbar/T)$, where $T$ is the period of a periodic orbit. We are primarily interested in the contribution of periodic orbits and will therefore largely ignore $\rho_{\rm TF}(E)$. One should keep in mind, however, that the Thomas-Fermi contribution should be included in the trace formulas that we will derive in this paper.

The stationary phase points of Eq. (2.8) that lie on a periodic orbit are not isolated, because, given any such point $\bar{\mathbf{z}}$, a nearby point on the same periodic orbit will also satisfy the stationary phase condition. Therefore the stationary phase points occur in families that are at least one dimensional. In his original derivation [1], Gutzwiller considered the most typical case in which each periodic orbit is isolated in its energy shell, so that the corresponding family of stationary phase points is precisely one dimensional. More generally, however, for example, when there are continuous symmetries present, periodic orbits may occur in higher-dimensional families, so that the stationary phase integrals are more degenerate. We will present a calculation of $g(E)$ that is valid in this more general case.

We assume that the periodic orbits occur in $k$-parameter families, so that a given family of periodic orbits maps out a $(1+k)$-dimensional surface in phase space, which we denote by $\Gamma$. In computing the integral over $\bar{\mathbf{z}}$ in Eq. (2.8), we will then split the $2n$ coordinates $\bar{\mathbf{z}}$ into a group of $1+k$ coordinates $\eta$, and a group of $2n-1-k$ coordinates $\zeta$—for example, we might let $\eta$ consist of the first $1+k$ components of $\mathbf{x}'$ and let $\zeta$ consist of the remaining $\mathbf{x}'$ components, along with all $n$ components of $\mathbf{p}$. For the moment, however, we let $\zeta$ and $\eta$ be quite arbitrary combinations of $\mathbf{x}'$ and $\mathbf{p}$ components. We will specify them in more detail later. Integrating over the $\zeta$ coordinates first, we find that the phase in Eq. (2.8) becomes rapidly varying away from the discrete set of $\zeta$ values (at fixed $\eta$) that corresponds to the periodic orbit family, allowing us to compute this part of integral by means of the standard stationary phase approximation. Having done this, we are left with a $(1+k)$-dimensional integral over $\Gamma$ in the $\eta$ coordinates, for which the phase is stationary and which must therefore be computed without approximation.

Carrying out explicitly the procedure outlined above, we arrive at the following sum over periodic orbit families $\Gamma$:

$$\begin{aligned} g(E)&\approx\frac{1}{i\hbar}\frac{1}{(2\pi\hbar)^{n-1/2}}\sum_{\Gamma}\int_{\Gamma}d\eta\left|\left[\frac{\partial(\mathbf{p}',t)}{\partial(\mathbf{p},E)}\right]_{\mathbf{x}'}\right|^{1/2}\exp\left[\frac{i}{\hbar}S(E)-i\mu\pi/2+i\nu\pi/4\right]\int d\zeta\exp\left[\frac{i}{2\hbar}\zeta\frac{\partial^2 S}{\partial\zeta\,\partial\zeta}\zeta\right] \\ &=\frac{1}{i\hbar}\frac{1}{(2\pi\hbar)^{k/2}}\sum_{\Gamma}\exp\left[\frac{i}{\hbar}S(E)-i\mu\pi/2+i\bar{\nu}\pi/4\right]\int_{\Gamma}d\eta\left|\left[\frac{\partial(\mathbf{p}',t)}{\partial(\mathbf{p},E)}\right]_{\mathbf{x}'}\right|^{1/2}\left|\frac{\partial^2 S}{\partial\zeta\,\partial\zeta}\right|^{-1/2}\ , \end{aligned} \tag{2.11}$$

where $\bar{\nu}=\nu+N_+-N_-$, and where $N_+$ and $N_-$ are, respectively, the number of positive eigenvalues and the number of negative eigenvalues of the $(2n-1-k)\times(2n-1-k)$ symmetric matrix $\partial^2 S/\partial\zeta\,\partial\zeta$ (derivatives with respect to $\zeta$ are taken while $\eta$ is held fixed). In particular, $N_++N_-=2n-1-k$. We have assumed that $\mu-\bar{\nu}/2$ is constant over $\Gamma$. It is convenient to rewrite $\mu-\bar{\nu}/2=\sigma+k/2$, where $\sigma=\mu-n+N_-+(1-\nu)/2$ is an integer.

We denote by $S(E)$ the value of $S(\mathbf{p},\mathbf{x}',E)$ on a periodic orbit. Because $S(\mathbf{p},\mathbf{x}',E)$ is stationary at periodic orbits, as in Eq. (2.9), $S(E)$ is the same for all periodic orbits in $\Gamma$, which is why it was removed from the integral in Eq. (2.11). We can express $S(E)$ in a more familiar form as follows:

$$S(E)=\oint -x\cdot d\mathbf{p}=\oint\mathbf{p}\cdot d\mathbf{x}\ , \tag{2.12}$$

where the integral is taken around any periodic orbit in $\Gamma$.

We can rewrite Eq. (2.11) as

$$g(E)\approx\frac{1}{i\hbar}\frac{1}{(2\pi i\hbar)^{k/2}}\sum_{\Gamma}A(\Gamma)\exp\left[\frac{i}{\hbar}S(E)-i\sigma\pi/2\right], \tag{2.13}$$

where the amplitude $A(\Gamma)$ is given by

$$A(\Gamma)=\int_{\Gamma}d\eta\left|\left[\frac{\partial(\mathbf{p}',t)}{\partial(\mathbf{p},E)}\right]_{\mathbf{x}'}\right|^{1/2}\left|\frac{\partial^2 S}{\partial\zeta\,\partial\zeta}\right|^{1/2}\ . \tag{2.14}$$

Thus each periodic orbit family contributes to $\rho(E)$ an oscillatory term whose phase is $S(E)$ and whose amplitude is $A(\Gamma)$. If we think of $\eta$ as local coordinates on $\Gamma$,

the amplitude $A(\Gamma)$ can be regarded as the total measure of $\Gamma$ with respect to a certain $(1+k)$-dimensional volume element $d\tau$, given by the integrand of Eq. (2.14). As it stands, this expression for $A(\Gamma)$ is rather difficult to interpret. The main object of the calculations from here on will be to find a more elegant interpretation of $A(\Gamma)$ in terms of intrinsic properties of $\Gamma$ that are easily determined in practice. The first step in making progress in this program is to decide on coordinates $\eta$ and $\zeta$.

So far, we have not specified in detail how $\eta$ and $\zeta$ are to be chosen. An important consideration in doing so is whether $1+k \leq n$ or $1+k > n$. For the Abelian symmetries we consider in this paper, we necessarily have $1+k \leq n$, so we treat this case here. We wish to point out, however, that this is not always the case for more complicated symmetries—for example, $k+1=3+1>n=3$ for a three-degree-of-freedom system with rotational symmetry—so the case $1+k>n$ will also need to be considered in general. As mentioned previously, one possible choice is to let $\eta$ consist of the first $1+k$ components of $\mathbf{x}'$ and to let $\zeta$ consist of the remaining components of $\mathbf{x}'$ and $\mathbf{p}$. While this choice will be perfectly good, in general, it is convenient to be more specific about the configuration-space coordinates. We use configuration-space coordinates $\mathbf{x}=(\mathbf{x}_\parallel,\mathbf{x}_\perp)$, constructed so that the coordinate axes of the $1+k$ coordinates $\mathbf{x}_\parallel$ are parallel to the periodic orbit family in configuration space and the coordinate axes of the remaining $n-1-k$ coordinates $\mathbf{x}_\perp$ are transverse to it, as shown in Fig. 1. In particular, the periodic orbit orbit family is at constant $\mathbf{x}_\perp$. Also, denote the momenta conjugate to $\mathbf{x}_\parallel$ and $\mathbf{x}_\perp$ by $\mathbf{p}_\parallel$ and $\mathbf{p}_\perp$, respectively. We then let $\eta=\mathbf{x}'_\parallel$ and $\zeta=(\mathbf{x}'_\perp,\mathbf{p})$.

Writing out the matrix $\partial^2 S/\partial\zeta\,\partial\zeta$ explicitly in terms of these coordinates and using the relationships in Eq. (2.9), we find

$$\begin{aligned}\left|\frac{\partial^2 S}{\partial\zeta\,\partial\zeta}\right| &= \begin{vmatrix} \dfrac{\partial^2 S}{\partial\mathbf{x}'_\perp\partial\mathbf{x}'_\perp} & \dfrac{\partial^2 S}{\partial\mathbf{p}\,\partial\mathbf{x}'_\perp} \\ \dfrac{\partial^2 S}{\partial\mathbf{x}'_\perp\partial\mathbf{p}} & \dfrac{\partial^2 S}{\partial\mathbf{p}\,\partial\mathbf{p}} \end{vmatrix} \\ &= \begin{vmatrix} \dfrac{\partial(\mathbf{p}_\perp-\mathbf{p}'_\perp)}{\partial\mathbf{x}'_\perp} & \dfrac{\partial(\mathbf{p}_\perp-\mathbf{p}'_\perp)}{\partial\mathbf{p}} \\ \dfrac{\partial(\mathbf{x}'-\mathbf{x})}{\partial\mathbf{x}'_\perp} & \dfrac{\partial(\mathbf{x}'-\mathbf{x})}{\partial\mathbf{p}} \end{vmatrix} \\ &= \left|\left[\frac{\partial(\mathbf{p}_\perp-\mathbf{p}'_\perp,\mathbf{x}-\mathbf{x}')}{\partial(\mathbf{x}'_\perp,\mathbf{p})}\right]_{\mathbf{x}'_\parallel,E}\right| \\ &= \left|\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}_\parallel,\mathbf{x}'_\parallel,E)}{\partial(\bar{\mathbf{z}},E)}\right]\right|, \end{aligned} \tag{2.15}$$

where we denote $\mathbf{z}_\perp=(\mathbf{x}_\perp,\mathbf{p}_\perp)$ and $\mathbf{z}_\parallel=(\mathbf{x}_\parallel,\mathbf{p}_\parallel)$. In the third line of the equation, we have used some rules for manipulating Jacobians that are outlined in more detail in Appendix A. Also, it may be helpful to note that we can replace $\mathbf{x}_\parallel-\mathbf{x}'_\parallel$ with $\mathbf{x}_\parallel$ in the numerator of these Jacobians because $\mathbf{x}'_\parallel$ is held fixed while the derivatives are taken. We can use Eq. (2.15) to combine the two factors in the integrand of Eq. (2.14) as follows:

$$\begin{aligned}\left|\left[\frac{\partial(\mathbf{p}',t)}{\partial(\mathbf{p},E)}\right]_{\mathbf{x}'}\right|^{1/2}\left|\frac{\partial^2 S}{\partial\zeta\,\partial\zeta}\right|^{-1/2} &= \left|\left[\frac{\partial(\mathbf{z}',t)}{\partial(\bar{\mathbf{z}},E)}\right]\right|^{1/2}\left|\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}_\parallel,\mathbf{x}'_\parallel,E)}{\partial(\bar{\mathbf{z}},E)}\right]\right|^{-1/2} \\ &= \left|\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}_\parallel,\mathbf{x}'_\parallel E)}{\partial(\mathbf{z}',t)}\right|^{-1/2} \\ &= \left|\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}_\parallel,E)}{\partial(\mathbf{z}'_\perp,\mathbf{p}'_\parallel,t)}\right]_{\mathbf{x}'_\parallel}\right|^{-1/2}. \end{aligned} \tag{2.16}$$

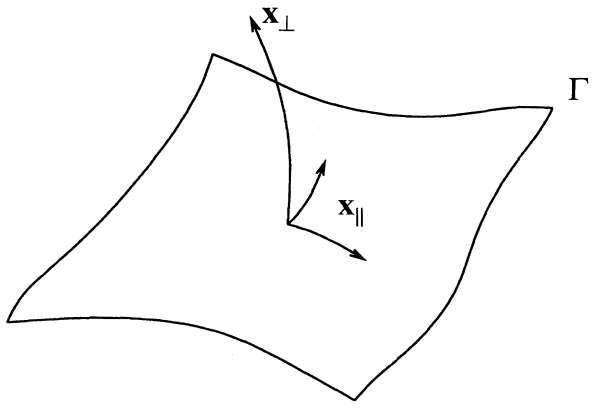


FIG. 1. The configuration space coordinates $(\mathbf{x}_\parallel,\mathbf{x}_\perp)$ are illustrated schematically for the case $k=1$. The $\mathbf{x}_\parallel$ coordinates are parallel to $\Gamma$ and the $\mathbf{x}_\perp$ coordinates transverse to $\Gamma$ in configuration space.

Finally, we can write for the amplitude $A(\Gamma)$

$$A(\Gamma)=\int_\Gamma d\mathbf{x}_\parallel\left|\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}_\parallel,E)}{\partial(\mathbf{z}'_\perp,\mathbf{p}'_\parallel,t)}\right]_{\mathbf{x}'_\parallel}\right|^{-1/2}. \tag{2.17}$$

Equation (2.17) is the final result of this section and is as far as we can take the calculations without making more detailed assumptions about the dynamics. Once again, we would like to stress that so far we have made no assumptions about the symmetries that are present other than $1+k \leq n$. In Sec. III we will assume that the periodic orbits occur in continuous families because of the presence of some number of first integrals in involution and we will use the ensuing symmetry to reduce $A(\Gamma)$ to a form in which it is easily computed in practice.

## III. USING THE SYMMETRY

From now on we will suppose that, in addition to the Hamiltonian $H$, there are $k$ independent constants of the motion $(J_1, \ldots, J_k)$, denoted collectively by $\mathbf{J}$, and that these constants are in involution. That is, we assume that any two first integrals $J_a$ and $J_b$ Poisson-commute as follows:

$$\{J_a, J_b\} = 0 \ . \tag{3.1}$$

We also assume that there are no other first integrals besides $\mathbf{J}$, so that the $J$'s account for all of the symmetry that is present in $H$. A particular example is that of axial symmetry, for which we can take $J = L_z$, the component of angular momentum along the symmetry axis. On the other hand, full three-dimensional rotational symmetry does not fall into this class, because two different components of angular momentum will not commute as in Eq. (3.1).

An important aspect of the presence of first integrals is that their existence is equivalent to the presence of a symmetry group for the Hamiltonian [18,19]. We can generate a symmetry of $H$ by letting phase space flow along the Hamiltonian vector field of any one of the constants, $J_a$ say, for an elapsed parameter $\theta_a$. Let us denote the symplectic mapping of phase space obtained in this way by $h_{\theta_a}$. Because $\{H, J_a\} = 0$, we see that $h_{\theta_a}$ preserves $H$ and that $h_{\theta_a}$ commutes with $\phi_t$, the flow of Hamiltonian $H$ for time $t$. Therefore $h_{\theta_a}$ is a symmetry of $H$. In this way, each $J_a$ generates a one-parameter symmetry group of $H$. Because of Eq. (3.1), the symmetries $h_{\theta_a}$ and $h_{\theta_b}$ generated by two different first integrals will commute [18]. Therefore the first integrals $\mathbf{J}$ will collectively generate an Abelian symmetry group, $G$ say, which is conveniently parametrized in terms of the $k$ vector $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_k)$. The vector $\boldsymbol{\theta}$ defines the transformation

$$h_{\boldsymbol{\theta}} = h_{\theta_1} \cdots h_{\theta_k} \ , \tag{3.2}$$

in which the ordering of the individual $h_{\theta_a}$ factors does not matter. Notice that $G$ is a $k$-dimensional group. One more consequence of Eq. (3.1) is that $\mathbf{J}$ is constant along $h_{\boldsymbol{\theta}}$ orbits, that is, $G$ preserves $\mathbf{J}$ as well as $H$. We note in passing that it will often be possible to choose the $J$'s in such a way that the $\boldsymbol{\theta}$ coordinates on $G$ are naturally $2\pi$ periodic; however, this will not always be the case.

Let us now examine the consequences of this symmetry for the structure of periodic orbits. From a given periodic orbit $\gamma_0$, the group $G$ will generate a $k$-parameter family of periodic orbits, all of the same energy and period. We can use $\boldsymbol{\theta}$ to parametrize this family of periodic orbits according to $\gamma_{\boldsymbol{\theta}}(t) = h_{\boldsymbol{\theta}} \gamma_0(t)$, as illustrated in Fig. 2. Because we assume that $G$ accounts for all of the symmetries of $H$, there are no other periodic orbits that are continuously related to a given $\gamma_{\boldsymbol{\theta}}$ except those generated by $G$. Therefore the whole family of periodic orbits $\Gamma$ is described naturally by the coordinates $(t, \boldsymbol{\theta})$. These coordinates give rise to a natural measure on $\Gamma$, defined by the volume element $dt\, d\boldsymbol{\theta}$. It will turn out, as one might expect, that the volume element $d\tau$, given by the integrand

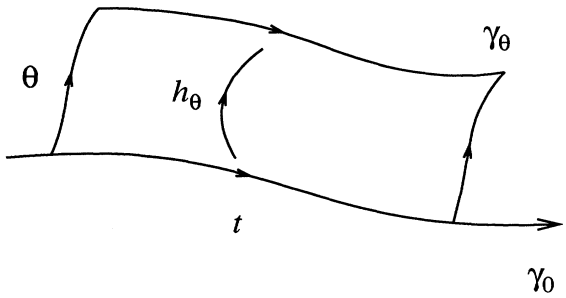


FIG. 2. The periodic orbit family $\Gamma$ is parametrized by $(t, \boldsymbol{\theta})$ through $\gamma_{\boldsymbol{\theta}}(t) = h_{\boldsymbol{\theta}} \gamma_0(t)$, illustrated here for $k = 1$.

of Eq. (2.16), is most naturally expressed in terms of $dt\, d\boldsymbol{\theta}$. In fact we will show that $d\tau$ is proportional to $dt\, d\boldsymbol{\theta}$, so that the integral for $A(\Gamma)$ in Eq. (2.16) is proportional to the total measure of $\Gamma$ with respect to the volume element $dt\, d\boldsymbol{\theta}$.

The coordinates described above are already somewhat familiar in the special case of integrable systems, for which $1 + k = n$. In this case $\Gamma$ is a rational torus, on which natural coordinates are given by the angle variables (which are not the same as $\boldsymbol{\theta}$). The coordinates $(\boldsymbol{\theta}, t)$ are then related to the angle coordinates by a constant linear transformation. In a similar vein we mention that, just as the invariant surfaces of integrable systems are topologically equivalent to $n$ tori [18], the periodic orbit families $\Gamma$ induced by Abelian symmetries are in general topologically equivalent to $(1+k)$ tori, provided they are compact (as must be the case for bound systems). This follows from the fact that any compact surface on which there exists a set of vector fields (in our case the Hamiltonian vector fields of $H$ and $\mathbf{J}$), that span the surface everywhere and that commute in the sense of the Lie bracket, is topologically a torus [18].

Let us now return to the program of converting Eq. (2.17) into a more usable form. As it stands, we can think of the Jacobian in Eq. (2.17) as corresponding to a change between alternate sets of coordinates, $(\mathbf{z}_\perp - \mathbf{z}'_\perp, \mathbf{x}'_\parallel, \mathbf{x}_\parallel, E)$ and $(\mathbf{z}'_\perp, \mathbf{x}'_\parallel, \mathbf{p}'_\parallel, t)$, on extended phase space $\mathcal{P} = P \times \mathbb{R}$. ($P$ is phase space and $\mathbb{R}$ corresponds to time.) Let us extend this idea a little further to include $\boldsymbol{\theta}$ evolution and consider the generalized extended phase space $\tilde{\mathcal{P}} = P \times \mathbb{R} \times \mathbb{R}^k$. Dynamics on generalized extended phase space is given by

$$(\mathbf{z}', t', \boldsymbol{\theta}') \rightarrow (\mathbf{z} = h_{\boldsymbol{\theta}} \phi_t \mathbf{z}', t + t', \boldsymbol{\theta} + \boldsymbol{\theta}')$$

in "time" $(t, \boldsymbol{\theta})$. We will generally take $t' = 0$ and $\boldsymbol{\theta}' = 0$. The obvious coordinates for $\tilde{\mathcal{P}}$ are $(\mathbf{z}, t, \boldsymbol{\theta})$ defined in the natural way. However, we will also be interested in coordinates $(\mathbf{z}', t, \boldsymbol{\theta})$, where $\mathbf{z}'$ is defined through $\mathbf{z} = h_{\boldsymbol{\theta}} \phi_t \mathbf{z}'$, and even coordinate systems that mix functions of $\mathbf{z}'$ (which we will always prime, as in $\mathbf{x}'_\parallel$, $\mathbf{p}'_\parallel$, etc.) and functions of $\mathbf{z}$.

In addition we note that from the extended-phase-space construction above and in the forthcoming calculations, it will become apparent that in many ways there is a symmetry between $t$ and $\boldsymbol{\theta}$ evolutions and between the Hamiltonian $H$ and the Hamiltonians $\mathbf{J}$. For example, we

have already seen that $t$ and $\theta$ appear symmetrically in the volume element $dt\,d\theta$. While this holds true for many aspects of the calculation, the final result must ultimately break the symmetry between $t$ and $\theta$ because we are calculating the density of states in energy, and this singles out the Hamiltonian $H$ from the other constants $\mathbf{J}$.

Using the generalized extended-phase-space construction above, we can reinterpret the integrand of Eq. (2.17) as a Jacobian on $\tilde{\mathcal{P}}$ as follows:

$$\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}_\parallel,E)}{\partial(\mathbf{z}'_\perp,\mathbf{p}'_\parallel,t)}\right]_{\mathbf{x}'_\parallel}\Bigg|_{\mathcal{P}}=\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}_\parallel,E)}{\partial(\mathbf{z}'_\perp,\mathbf{p}'_\parallel,t)}\right]_{\mathbf{x}'_\parallel,\theta}\Bigg|_{\tilde{\mathcal{P}}}$$
$$=\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E,\theta)}{\partial(\mathbf{z}'_\perp,\mathbf{z}'_\parallel,t,\theta)}\,, \tag{3.3}$$

where of course we evaluate these Jacobians for the particular evolution parameters $\theta=0$ and $t=T$, the period of the periodic orbit. Notice that the Jacobian of Eq. (3.3) involves only time evolution. We will now do some manipulations that lead to derivatives with respect to $\theta$ (evaluated at $\theta=0$), and these will introduce infinitesimal $\theta$ evolutions into the calculation. We use the chain rule to expand the Jacobian into the following product:

$$\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E,\theta)}{\partial(\mathbf{z}'_\perp,\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E,\mathbf{J})}\right]\left[\frac{\partial(\mathbf{z}'_\perp,\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E,\mathbf{J})}{\partial(\mathbf{z}'_\perp,\mathbf{z}'_\parallel,t,\theta)}\right]$$
$$=\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\theta)}{\partial(\mathbf{z}'_\perp,\mathbf{J})}\right]_{\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E}\left[\frac{\partial(\mathbf{x}_\parallel,E,\mathbf{J})}{\partial(\mathbf{p}'_\parallel,t,\theta)}\right]_{\mathbf{z}'_\perp,\mathbf{x}'_\parallel}. \tag{3.4}$$

Because $h_\theta\phi_t$ preserves $\mathbf{J}$, the value of $\mathbf{J}$ appearing above can refer either to the initial point $\mathbf{z}'$ or the final point $\mathbf{z}$.

Let us concentrate on the second Jacobian in Eq. (3.4). Using the chain rule we break it up as follows:

$$\left[\frac{\partial(\mathbf{x}_\parallel,E,\mathbf{J})}{\partial(\mathbf{p}'_\parallel,t,\theta)}\right]_{\mathbf{z}'_\perp,\mathbf{x}'_\parallel}=\left[\frac{\partial(\mathbf{x}_\parallel,E,\mathbf{J})}{\partial(t,\theta,E,\mathbf{J})}\right]_{\mathbf{z}'_\perp,\mathbf{x}'_\parallel}\left[\frac{\partial(t,\theta,E,\mathbf{J})}{\partial(\mathbf{p}'_\parallel,t,\theta)}\right]_{\mathbf{z}'_\perp,\mathbf{x}'_\parallel}$$
$$=\left[\frac{\partial(\mathbf{x}_\parallel)}{\partial(t,\theta)}\right]_{\mathbf{z}'_\perp,\mathbf{x}'_\parallel,E,\mathbf{J}}\left[\frac{\partial(E,\mathbf{J})}{\partial(\mathbf{p}'_\parallel)}\right]_{\mathbf{z}'_\perp,\mathbf{x}'_\parallel,t,\theta}$$
$$=\left[\frac{\partial(\mathbf{x}_\parallel)}{\partial(t,\theta)}\right]_{\mathbf{z}'}\left[\frac{\partial(E,\mathbf{J})}{\partial(\mathbf{p}'_\parallel)}\right]_{\mathbf{z}'_\perp,\mathbf{x}'_\parallel,t,\theta}. \tag{3.5}$$

In the second line of the equation we have used the fact that fixing $(\mathbf{z}'_\perp,\mathbf{x}'_\parallel,E,\mathbf{J})$ is equivalent to fixing $\mathbf{z}'$ (recall that $E=E'$ and $\mathbf{J}=\mathbf{J}'$). By invoking Hamilton's equations, we can see that the two final Jacobians in Eq. (3.5) are, in fact, equal to each other on $\Gamma$. The first is given by a matrix of $\mathbf{x}_\parallel$ velocities under Hamiltonians $(H,\mathbf{J})$, evaluated at $\mathbf{z}$. By Hamiltonian's equations, the second is given by a matrix of $\mathbf{x}_\parallel$ velocities evaluated at $\mathbf{z}'$. When $\mathbf{z}=\mathbf{z}'$ both of these Jacobians are equal. Each of the Jacobians, when evaluated on $\Gamma$, can be thought of as a Jacobian for the change of coordinates, $(t,\theta)$ to $\mathbf{x}_\parallel$, on $\Gamma$. This is because the Hamiltonian flow vectors for the Hamiltonians $(H,\mathbf{J})$ are coordinate basis vectors for the coordinates $(t,\theta)$ on $\Gamma$. We can therefore write

$$d\mathbf{x}_\parallel\left|\left[\frac{\partial(\mathbf{x}_\parallel,E,\mathbf{J})}{\partial(\mathbf{p}'_\parallel,t,\theta)}\right]_{\mathbf{z}'_\perp,\mathbf{x}'_\parallel}\right|^{-1/2}=d\mathbf{x}_\parallel\left|\left[\frac{\partial(\mathbf{x}_\parallel)}{\partial(t,\theta)}\right]_\Gamma^2\right|^{-1/2}$$
$$=d\mathbf{x}_\parallel\left|\frac{\partial(t,\theta)}{\partial(\mathbf{x}_\parallel)}\right|$$
$$=dt\,d\theta\,. \tag{3.6}$$

We have reduced the amplitude $A(\Gamma)$ to the following form:

$$A(\Gamma)=\int_\Gamma dt\,d\theta\left|\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\theta)}{\partial(\mathbf{z}'_\perp,\mathbf{J})}\right]_{\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E}\right|^{-1/2}. \tag{3.7}$$

Once again we use the chain rule to break up the remaining Jacobian,

$$\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\theta)}{\partial(\mathbf{z}'_\perp,\mathbf{J})}\right]_{\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E}=\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\theta)}{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{J})}\right]_{\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E}\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp,\mathbf{J})}{\partial(\mathbf{z}'_\perp,\mathbf{J})}\right]_{\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E}$$
$$=\left[\frac{\partial\theta}{\partial\mathbf{J}}\right]_{\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E,\mathbf{z}_\perp-\mathbf{z}'_\perp}\left[\frac{\partial(\mathbf{z}_\perp-\mathbf{z}'_\perp)}{\partial\mathbf{z}'_\perp}\right]_{\mathbf{x}'_\parallel,\mathbf{x}_\parallel,E,\mathbf{J}}. \tag{3.8}$$

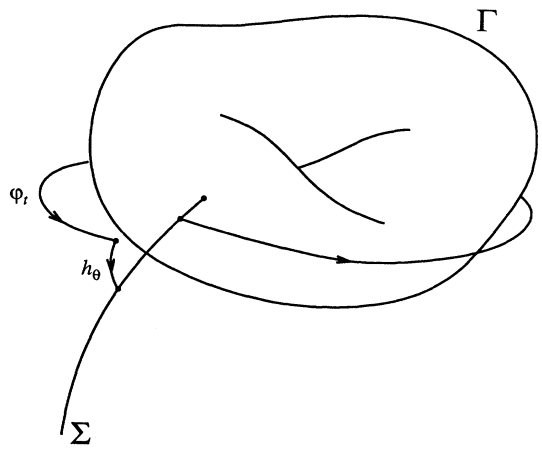


FIG. 3. A schematic illustration of the construction of the reduced surface of section considered in Sec. III, in which some dimensions have been suppressed. The picture is meant to be embedded in a surface of constant $(H,\mathbf{J})$. A trajectory starting on $\Sigma$ is first carried around $\Gamma$ with $\phi_t$, and subsequently projected back onto $\Sigma$ with $h_\theta$. In this way a mapping $\psi$: $\Sigma\to\Sigma$ is obtained. There is no special significance to the curves drawn on $\Gamma$ here. They are just meant to represent folds and tucks, allowing for $\Gamma$ to have nontrivial topology.

These Jacobians are very conveniently interpreted in terms of the dynamics on a reduced surface of section, which arises in the following way. Consider the second Jacobian, whose derivatives are taken at constant $(\mathbf{x}'_{\|},\mathbf{x}_{\|},E,\mathbf{J})$. To evaluate this we consider trajectories whose initial conditions are displaced from $\Gamma$ at constant $\mathbf{x}_{\|}$ and constant $(H,\mathbf{J})$. After following one of these trajectories around $\Gamma$ we then adjust $t$ and $\boldsymbol{\theta}$ until the trajectory returns to the original value of $\mathbf{x}_{\|}$. Because we have assumed that $G$ preserves $\mathbf{J}$, this trajectory ends up with the same values of $(H,\mathbf{J})$ that it started with. The process we have just described, designed so that the derivatives are taken at constant $(\mathbf{x}'_{\|},\mathbf{x}_{\|},E,\mathbf{J})$, describes exactly a surface of section mapping on a reduced surface of section $\Sigma=\{\mathbf{z}|\mathbf{x}_{\|},H,\mathbf{J}=\text{const}\}$, illustrated in Fig. 3. It is just like a regular surface of section mapping except that $\Sigma$ is codimension $k+1$ in the invariant surface $\{\mathbf{z}|H,\mathbf{J}=\text{const}\}$, rather than codimension 1 in the invariant surface $\{\mathbf{z}|H=\text{const}\}$, and we vary $k+1$ parameters $(t,\boldsymbol{\theta})$, rather than 1 parameter $t$, to get trajectories back to $\Sigma$. (In Appendix B we make a listing of the differences between the various structures that contribute to the trace formula and make a comparison between systems with symmetry and systems without symmetry, so it might be convenient to refer there at appropriate points in this section.) Let us denote the mapping by $\psi$. Since $\Sigma$ is even dimensional, we can make it into a symplectic manifold by restricting the full-phase-space symplectic form $\Omega$ to it. It is shown in Appendix C that $\psi$ is symplectic with respect to this symplectic structure.

Denote the linearization of $\psi$ at the periodic orbit by $M$. We can use coordinates $\mathbf{z}_{\perp}$ on $\Sigma$, in terms of which the $2(n-1-k)\times 2(n-1-k)$ matrix $M$ can be written

$$M=\left.\frac{\partial \mathbf{z}_{\perp}}{\partial \mathbf{z}'_{\perp}}\right|_{\Sigma} . \tag{3.9}$$

This allows us to write

$$\left.\frac{\partial(\mathbf{z}_{\perp}-\mathbf{z}'_{\perp})}{\partial \mathbf{z}'_{\perp}}\right|_{\mathbf{x}'_{\|},\mathbf{x}_{\|},E,\mathbf{J}}=\left.\frac{\partial \mathbf{z}_{\perp}}{\partial \mathbf{z}'_{\perp}}\right|_{\Sigma}-I=M-I . \tag{3.10}$$

This is just like the factor that arises in Gutzwiller's formula for isolated orbits, except that here $M$ is the linearization of a reduced surface of section mapping rather than a regular surface of section mapping.

An important point is that the quantity of interest for Eq. (3.7), $\det(M-I)$, is an invariant of $\Gamma$. We can see this as follows. First, we are free to compute $M$ in terms of any set of coordinates on $\Sigma$ besides $\mathbf{z}_{\perp}$ (even noncanonical coordinates). This is because the effect of a change of coordinates is to conjugate $M$ with the Jacobian matrix of the coordinate change, which leaves $\det(M-I)$ invariant. Second, we find, for similar reasons, that $\det(M-I)$ remains unchanged if we compute it for a different surface of section $\Sigma'$, even if $\Sigma'$ is located at a different point of $\Gamma$. To see this let $w$ be the mapping from $\Sigma$ to some nearby $\Sigma'$. Then the surface of section mapping for $\Sigma'$ is $\psi'=w\circ\psi\circ w^{-1}$, so that $M'$ is related to $M$ by conjugation and $\det(M'-I)=\det(M-I)$. The term $\det(M-I)$ is determined solely by the eigenvalues of $M$. As discussed in Appendix D, these eigenvalues are simultaneously eigenvalues of the linearization of the full-phase-space dynamics and may therefore be obtained without the use of a reduced surface of section mapping.

The remaining Jacobian $(\partial\boldsymbol{\theta}/\partial\mathbf{J})_{\mathbf{x}'_{\|},\mathbf{x}_{\|},E,\mathbf{z}_{\perp}-\mathbf{z}'_{\perp}}$ can also be given an invariant meaning in terms of reduced surface of section mappings. For this it is useful to allow the $\mathbf{J}$ at which the reduced surface of section is constructed to vary (but we still restrict ourselves to $H=E$). This creates a family of reduced surfaces of section $\Sigma_{\mathbf{J}}$, parametrized by $\mathbf{J}$. Keeping $(\mathbf{x}'_{\|},\mathbf{x}_{\|},E,\mathbf{z}_{\perp}-\mathbf{z}'_{\perp})$ fixed then amounts to following the fixed points of the maps $\psi_{\mathbf{J}}$ as $\mathbf{J}$ is varied. These fixed points lie on what we call generalized periodic orbits: trajectories which close on themselves after a generalized time $(\boldsymbol{\Theta},T)$. We call $(\boldsymbol{\Theta},T)$ the generalized period. As with ordinary periodic orbits, generalized periodic orbits arise in $(k+1)$-dimensional families, which we denote $\Gamma_{\mathbf{J}}$. (We will still use the simpler notation $\Gamma$ for the ordinary periodic orbits.) Near $\Gamma$ there is precisely one $\Gamma_{\mathbf{J}}$ for each $\mathbf{J}$. We can then interpret $(\partial\boldsymbol{\theta}/\partial\mathbf{J})_{\mathbf{x}'_{\|},\mathbf{x}_{\|},E,\mathbf{z}_{\perp}-\mathbf{z}'_{\perp}}$ as the Jacobian for a change from $\mathbf{J}$ to $\boldsymbol{\Theta}$ as labels of $\Gamma_{\mathbf{J}}$,

$$\left.\frac{\partial\boldsymbol{\theta}}{\partial\mathbf{J}}\right|_{\mathbf{x}'_{\|},\mathbf{x}_{\|},E,\mathbf{z}_{\perp}-\mathbf{z}'_{\perp}}=\left.\frac{\partial\boldsymbol{\Theta}}{\partial\mathbf{J}}\right|_{\Gamma_{\mathbf{J}}=\Gamma} . \tag{3.11}$$

Because $\boldsymbol{\Theta}$ is constant on each $\Gamma_{\mathbf{J}}$, the Jacobian on the right is well defined, and in fact is itself constant on $\Gamma$. The Jacobian $\partial\boldsymbol{\Theta}/\partial\mathbf{J}$ is actually quite easily computed once a linearization of the full-phase-space dynamics is found. We outline how this is done in Appendix D.

We have shown that the integrand of Eq. (3.7) is constant, so we can write

$$A(\Gamma)=|\det(M-I)|^{-1/2}\left|\frac{\partial\boldsymbol{\Theta}}{\partial\mathbf{J}}\right|^{-1/2}\int_{\Gamma}dt\,d\boldsymbol{\theta} . \tag{3.12}$$

All that remains is to compute the volume of $\Gamma$ with respect to $dt\,d\boldsymbol{\theta}$. In the case of isolated orbits, there is only an integral over $t$, giving $T_0$, the period of the primitive periodic orbit, as in Gutzwiller's formula. More generally, we are left with a $\boldsymbol{\theta}$ integral after integrating over $t$. To examine this we use a construction that is related to the discussion of Arnol'd in Ref. [18], p. 274, so we refer the reader there for more details. First we identify points in $\boldsymbol{\theta}$ space which map $\gamma_0$ into itself. In doing so we get a lattice of points in $\boldsymbol{\theta}$ space, in which we can identify a unit cell with the $k$ torus that one obtains in a constant time slice of $\Gamma$. The integral over $\boldsymbol{\theta}$ is then just the $k$ volume $V_0$ of a unit cell. If $(e_1,\ldots,e_k)$ are basis vectors for the lattice we can write

$$\int d\boldsymbol{\theta}=V_0=\det(e_1,\ldots,e_k) . \tag{3.13}$$

Equation (3.13) reduces the integral of Eq. (3.12) to the discrete calculation of finding $T_0$ and $(e_1,\ldots,e_k)$, and then taking a determinant.

We have now fulfilled the task of expressing $A(\Gamma)$ in a coordinate-free, invariant way. We collect the results in the following trace formula:

$$g(E)\approx\frac{1}{i\hbar}\frac{1}{(2\pi i\hbar)^{k/2}}\sum_{\Gamma}\frac{T_0V_0\exp\left[\frac{i}{\hbar}S(E)-i\sigma\pi/2\right]}{\left|\frac{\partial\Theta}{\partial\mathbf{J}}\right|^{1/2}|\det(M-I)|^{1/2}}\,. \tag{3.14}$$

Expressed in this way, we see that the results are very much like Gutzwiller's trace formula for isolated orbits. Instead of a sum over individual orbits we have a sum over $k$ parameter families, each of whose contributions is enhanced by a factor of order $\hbar^{-k/2}$ over the contributions of isolated orbits in Gutzwiller's formula. The period of the primitive periodic orbit $T_0$ is replaced with $T_0V_0$ and $M$ is obtained from a reduced surface of section mapping rather than the regular surface of section mapping of Gutzwiller's formula. The only remaining difference is that an extra factor $|\partial\Theta/\partial\mathbf{J}|^{-1/2}$ appears that is not present in the sum for isolated orbits.

## IV. SPECIAL CASES

In this section we will illustrate the general results of Sec. III with some important special cases. In IV A we consider the case of axial symmetry, which is perhaps the simplest nontrivial example to which our results apply. In particular, we consider systems of three degrees of freedom, using as a primary example, the hydrogen atom in a strong magnetic field. In V B we go on to examine the case of integrable systems, where we reinterpret Eq. (3.14) in terms of action-angle variables.

### A. Axial symmetry

Let us examine how Eq. (3.14) applies to axially symmetric systems of three degrees of freedom. We use cylindrical polar coordinates $(\rho,\theta,z)$ on configuration space, with the conjugate momenta denoted by $(p_\rho,p_\theta,p_z)$. In cases of axial symmetry, the $\theta$ coordinate is ignorable in the Hamiltonian $H(\rho,z,p_\rho,p_\theta,p_z)$. We take as our model for such systems the example of a hydrogen atom in a strong magnetic field, for which the Hamiltonian can be put in the following dimensionless form [6,7]:

$$H(\rho,z,p_\rho,p_\theta,p_z)=\frac{1}{2}\left[p_\rho^2+\frac{p_\theta^2}{\rho^2}+p_z^2\right]-\frac{1}{r}+\frac{\gamma^2}{8}\rho^2\,, \tag{4.1}$$

where $r^2=\rho^2+z^2$ and $\gamma$ is proportional to the magnetic-field strength. This system is of interest because it is an example of an experimentally realized system that can exhibit global chaos in phase space.

The obvious way to deal with a Hamiltonian like that in Eq. (4.1) is to ignore the $\theta$ coordinate and treat $H(\rho,z,p_\rho,p_\theta,p_z)$ as a system of two-degree-of-freedom Hamiltonians, parametrized by $p_\theta$. This reduced physical system misses crucial information, however, which is required for the trace formula discussed in this paper. For example, periodic orbits of the reduced system will, in general, not close in the $\theta$ coordinate and so will not be periodic in the full system. While applying the trace formula to the reduced classical system does not lead to the full density of states, it does give a reduced density of states, corresponding to a magnetic quantum number of $m=p_\theta/\hbar$. This is the approach that has been taken with the system of Eq. (4.1) in the past, and has been quite successful [6,7]. However, besides being of academic interest, there are practical reasons for wanting to apply the trace formula to the full density of states. For example, it is the full density of states, not the partial densities of states, that is important for the shell structure in nuclei. Thus the results of this section are of interest for the shell structure of highly deformed nuclei.

The first step in applying Eq. (3.14) is to evaluate the action $S(E)$ of the periodic orbit. This is related to the action $\tilde{S}(E)=\oint p_\rho d\rho+p_z dz$ in the reduced system according to

$$S(E)=\tilde{S}(E)+\oint p_\theta d\theta\,. \tag{4.2}$$

Assuming that the periodic orbit winds around the axis of symmetry $N$ times, we have

$$S(E)=\tilde{S}(E)+2\pi NL_z\,, \tag{4.3}$$

where we use $L_z$ to denote the particular value of $p_\theta$ on the periodic orbit family.

Turning to the amplitude, it turns out that a regular surface of section mapping about the periodic orbit in reduced phase space can be used to evaluate the term $\det(M-I)$. Let us illustrate this for the particular example of a surface of section $\tilde{\Sigma}(z=0)$, formed in the reduced phase space by fixing $z=0$ and $H=E$ (while the process of reduction fixes $p_\theta=L_z$). Let $\tilde{\psi}$ denote the mapping on $\tilde{\Sigma}$. We will compare this with a mapping $\psi$ on a reduced surface of section $\Sigma$, constructed in the manner discussed in Sec. III. According to the theory presented there, $\Sigma$ is formed by fixing $H=E$, $p_\theta=L_z$ along with two additional parameters. In order to have $\Sigma$ correspond to $\tilde{\Sigma}$, one of the additional conditions must obviously be $z=0$. Let us choose the other condition to be $\theta=0$. We can use $(\rho,p_\rho)$ as coordinates on both $\tilde{\Sigma}$ and $\Sigma$—we will show that $\tilde{\psi}$ and $\psi$ are identical when written in these coordinates.

The surface of section mapping on $\tilde{\Sigma}$ is illustrated in Fig. 4. A trajectory is started at $z=0$ with $\dot{z}>0$ and is iterated forward until it passes through $z=0$ once again with $\dot{z}>0$. Denote this by $(\rho',p'_\rho)\rightarrow(\bar{\rho},\bar{p}_\rho)$. To map the corresponding point on $\Sigma$ using $\psi$, we start the same trajectory in full phase space, but with the additional initial condition $\theta'=0$. We must now use both time evolution and rotation to bring this trajectory back to $z=0$ and $\theta=0$. To do this we first follow the trajectory forward in time until it passes through $z=0$ with $(\rho,p_\rho)=(\bar{\rho},\bar{p}_\rho)$ and $\theta=\bar{\theta}$. Then this point is returned to $\theta=0$ by a rotation through angle $-\bar{\theta}$, completing the mapping $\psi$. Since $(\bar{\rho},\bar{p}_\rho)$ is constant under rotation (the Hamiltonian is $p_\theta$), we see that the mapping $\psi$ takes $(\rho',p'_\rho)$ into $(\bar{\rho},\bar{p}_\rho)$, so the mapping $\tilde{\psi}$ and $\psi$ are identical in these coordinates as claimed. Finally, we note that none of the arguments above were particular to the $z=0$ surface of section, so we assert that the mappings are equivalent in general.

We now consider the $T_0V_0$ factor. We expect that a generic periodic orbit will be mapped into itself by a rota-

tion of angle $2\pi$, but by no smaller rotation. Therefore we generally find that $T_0 V_0 = 2\pi T_0$. Exceptional cases can occur, however, in which the periodic orbit is symmetric under a smaller rotation, $2\pi/N_I$ say. $N_I$ counts the number of distinct rotations that map the periodic orbit into itself. Including these exceptional cases, we therefore have $T_0 V_0 = (2\pi/N_I) T_0$. We mention in passing that there might be periodic orbits that are even more degenerate in that they are invariant under all rotations. These correspond to equilibria of the reduced system. Periodic orbits such as these will be isolated in the full-phase-space energy shell and will contribute to the density of states at a lower order in $\hbar$ (their contribution is smaller by a factor of order $\hbar^{1/2}$) than regular orbits.

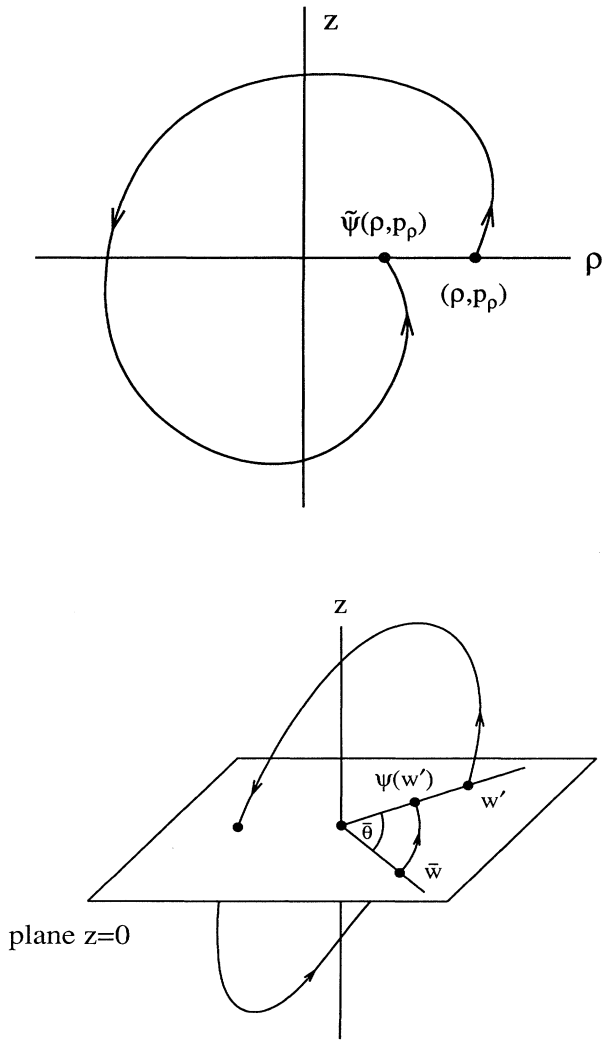


FIG. 4. A configuration-space picture of the surfaces of section $\tilde{\psi}$ and $\psi$ described in Sec. IV. In (a) the mapping $\tilde{\psi}$ is constructed in the reduced coordinates $(\rho,z)$ in the usual way. This is to be contrasted with (b), where we present the corresponding picture for the mapping $\psi$ in the full set of coordinates $(\rho,\theta,z)$. We first follow a trajectory starting at $z=0$ and $\theta=0$ (phase space point $w'$) until it passes through $z=0$ with $\dot{z}>0$ (at $\bar{w}$) and then rotate back to $\theta=0$ [giving $\psi(w')$] to complete the mapping.

The last remaining factor that needs to be dealt with is the $\partial\Theta/\partial\mathbf{J}$ term, in which $\Theta$ consists of a single component $\Theta$ and $\mathbf{J}=p_\theta$ for axial symmetry. $\Theta$ is the amount by which periodic orbits of the reduced system fail to close in the coordinate $\theta$, as a function of $p_\theta$. That is, given a point on a periodic orbit of the reduced system, a corresponding point in the full phase space will close on itself after some time evolution and a rotation through angle $\Theta$. We then have the following specialization for these systems:

$$\frac{\partial\Theta}{\partial\mathbf{J}} \sim \frac{d\Theta}{dp_\theta} . \tag{4.4}$$

Notice that this represents information that is missing in the reduced system, so full-phase-space dynamics is necessary to determine it. As discussed in Appendix D, it is not actually necessary to know directly about the generalized periodic orbits in order to evaluate Eq. (4.4). For that purpose a linearization of the full-phase-space dynamics about the genuinely periodic orbit will suffice.

We can now write a specialized trace formula for axially symmetric systems as follows:

$$g(E) \approx \frac{1}{i\hbar}\frac{1}{(2\pi i\hbar)^{1/2}} \times \sum_{\substack{\text{periodic}\\ \text{orbits}}} \frac{\frac{2\pi}{N_I} T_0 \exp\left[\frac{i}{\hbar}S(E) - i\sigma\pi/2\right]}{\left|\frac{d\Theta}{dp_\theta}\right|^{1/2} |\det(M-I)|^{1/2}} , \tag{4.5}$$

giving the complete density of states. Besides the fact that it sums over periodic orbits of the full phase space dynamics, Eq. (4.5) differs from the application of Eq. (1.1) to the reduced system (for the reduced dynamics) in the presence the term $d\Theta/dp_\theta$, which has no analog in Eq. (1.1). In addition, the phase $S(E)$ is slightly different, as indicated by Eq. (4.3).

Finally, we would like to point out that the considerations of this section are easily adjusted to apply to any system in which the symmetry manifests itself as the presence of ignorable coordinates.

### B. Integrable systems

Integrable systems form an important special case of the calculations presented in this paper, and the results for such systems are most naturally expressed in terms of action-angle variables $(\mathbf{I},\boldsymbol{\phi})$. It is therefore of interest to discuss how action-angle variables may be used to compute Eq. (3.14), as we do in this section. Our calculations will quickly converge to those of Berry and Tabor [14], who show (in reverse) how the trace formula may be summed for integrable systems to yield the torus quantization conditions.

Integrable systems correspond to the case $k+1=n$, in which there is a complete set of commuting observables. Using a standard procedure [18], one can use the $n$ first integrals $(H,\mathbf{J})$ to compute action-angle coordinates $(\mathbf{I},\boldsymbol{\phi})$ on phase space, which are canonical coordinates with the property that the Hamiltonian $H=H(\mathbf{I})$ is a function of

$\mathbf{I}$ alone, independent of $\phi$. The first integrals $\mathbf{J}=\mathbf{J}(\mathbf{I})$ can also be expressed as functions of $\mathbf{I}$ alone. The level sets of $\mathbf{I}$ are the invariant tori, which are invariant under $t$ and $\theta$ evolution. In fact, each invariant torus is the orbit under $(t,\theta)$ evolution of any point on that torus.

The periodic orbit families for integrable systems are precisely the rational tori, which we can label with $n$ vectors of integers, $N$, according to

$$\omega T=2\pi N\ , \tag{4.6}$$

where $T$ is the period and $\omega(\mathbf{I})=\partial H(\mathbf{I})/\partial\mathbf{I}$ is the vector of angular frequencies corresponding to action-angle variables $(\mathbf{I},\phi)$. The phase $S(E)$ entering into Eq. (3.14) can be expressed in terms of the actions as follows:

$$S(E)=2\pi\mathbf{N}\cdot\mathbf{I}\ , \tag{4.7}$$

where this follows immediately from the defining relationships for $\mathbf{I}$ or from direct computation of Eq. (2.12) in action-angle coordinates. Turning to the amplitude of Eq. (3.14), we note that the reduced surfaces considered in Sec. III are vacuous for integrable systems, so the factor $\det(M-I)$ is absent [as when Eq. (1.1) is applied to systems of one degree of freedom].

The remaining contributions to the trace formula need more consideration. It is convenient, rather than dealing with $\partial\Theta/\partial J$ directly in Eq. (3.14), to consider instead $\partial(T,\Theta)/\partial(H,\mathbf{J})$, which is related to $\partial\Theta/\partial\mathbf{J}$ through

$$\frac{\partial(T,\Theta)}{\partial(H,\mathbf{J})}=\frac{\partial(T,\Theta)}{\partial(H,\Theta)}\frac{\partial(H,\Theta)}{\partial(H,\mathbf{J})}=\frac{dT(E)}{dE}\left[\frac{\partial\Theta}{\partial\mathbf{J}}\right]_E\ , \tag{4.8}$$

where $T(E)$ is the period of the rational torus as a function of $E$. We can identify $(\partial T/\partial E)_\Theta=dT/dE$ because holding $\Theta$ fixed (at 0) is equivalent to fixing the winding number of a rational torus. Let us now consider the term

$$T_0V_0\left|\frac{\partial(T,\Theta)}{\partial(H,\mathbf{J})}\right|^{-1/2}=\int_\Gamma dt\,d\theta\left|\frac{\partial(T,\Theta)}{\partial(H,\mathbf{J})}\right|^{-1/2}\ . \tag{4.9}$$

As should be expected, $dt\,d\theta|\partial(T,\Theta)/\partial(H,\mathbf{J})|^{-1/2}$ is invariant under a redefinition of the first integrals $(H,\mathbf{J})$, and, in particular, it is invariant if we replace $(H,\mathbf{J})$ with the action variables $\mathbf{I}$. In this case the conjugate variables $(t,\theta)$ are replaced with $\phi$. The generalized period $(T,\Theta)$ is replaced by $\Phi(\mathbf{I})$, which is the angle displacement of an initial condition on the rational torus from its trajectory after a propagation for time $T$—this is just $2\pi\mathbf{N}-\omega(\mathbf{I})T$. In this expression, $T$ is fixed at the value it takes on the particular rational torus at the energy of interest. The volume element $dt\,d\theta$ is replaced by $d\phi$, which integrates to $(2\pi)^n$. We find therefore that

$$\begin{aligned}T_0V_0\left|\frac{\partial(T,\Theta)}{\partial(H,\mathbf{J})}\right|^{-1/2}&=(2\pi)^n\left|\frac{\partial\Phi}{\partial\mathbf{I}}\right|^{-1/2}\\&=(2\pi)^nT^{-n/2}\left|\frac{\partial\omega}{\partial\mathbf{I}}\right|^{-1/2}\ .\end{aligned} \tag{4.10}$$

It remains to express $dT(E)/dE$ of Eq. (4.8) directly in terms of action-angle variables. To do this we first differentiate Eq. (4.6) with respect to $E$ while holding $\mathbf{N}$ fixed, that is, we follow the rational torus labelled by $\mathbf{N}$ as a function of energy. This yields

$$\frac{\partial\omega(\mathbf{I})}{\partial\mathbf{I}}\cdot\frac{\partial\mathbf{I}}{\partial E}T+\omega\frac{dT}{dE}=0\ . \tag{4.11}$$

Differentiating $H(\mathbf{I})=E$ in the same way gives $1=\omega\cdot\partial\mathbf{I}/\partial E$, which can be used to eliminate $\partial\mathbf{I}/\partial E$ from Eq. (4.11). The result is

$$\frac{dT}{dE}=-\frac{T}{\omega\cdot D^{-1}\cdot\omega}\ , \tag{4.12}$$

where $D$ is the $n\times n$ symmetric matrix $\partial\omega/\partial\mathbf{I}=\partial^2H/\partial\mathbf{I}\,\partial\mathbf{I}$, assumed to be nonsingular.

This completes the calculation of the various terms contributing to Eq. (3.14). Collecting these results together, we arrive at the following trace formula for integrable systems:

$$g(E)=\frac{1}{i\hbar}\left[\frac{2\pi}{i\hbar}\right]^{n/2}\sum_{\substack{\text{rational}\\\text{tori}}}\frac{\exp\left[\dfrac{2\pi i\mathbf{N}\cdot\mathbf{I}}{\hbar}-\dfrac{i\sigma\pi}{2}\right]}{T^{n-1/2}|\det D|^{1/2}|\omega\cdot D^{-1}\cdot\omega|^{1/2}}\ . \tag{4.13}$$

Everything here is easily calculated once the action angle variables are known. From here one can follow directly the calculations of Berry and Tabor to recover the torus quantization rules. We refer the reader to their work [14] for further details.

## V. CONCLUSION

We can summarize the results of this paper with the following explicit formula for the oscillatory part of the density of states:

$$\rho_{\rm osc}(E)\approx\frac{1}{\pi\hbar}\frac{1}{(2\pi\hbar)^{k/2}}\sum_{\substack{\text{periodic}\\\text{orbit}\\\text{families}}}\frac{T_0V_0\cos\left[\dfrac{S}{\hbar}-\dfrac{\sigma\pi}{2}-\dfrac{k\pi}{4}\right]}{\left|\dfrac{\partial\Theta}{\partial\mathbf{J}}\right|^{1/2}|\det(M-I)|^{1/2}}\ . \tag{5.1}$$

This is a direct generalization of Eq. (1.1) and is obtained from the trace formula of Eq. (3.14) by a straightforward application of Eq. (2.2). Just like Gutzwiller's formula for isolated orbits, this trace formula depends on intrinsic properties of the periodic orbit families that are clearly independent of the coordinates used to compute them.

It remains to be seen that the Maslov index $\sigma$ occurring in the trace formula in this paper has an invariant geometrical interpretation. In the case of isolated periodic orbits, it has been shown [3,4] that the Maslov index is equal to the number of times that stable and unstable manifolds wind around the periodic orbit over one traversal of it. There should obviously be a similar interpretation for the index of Eq. (5.1), involving the invariant manifolds of the whole family $\Gamma$ (which are Lagrangian), though we have not shown that in this paper. Such an interpretation would be useful in a practical implementation of Eq. (6.1).

The calculations presented in this paper have generalizations to the case where there is a non-Abelian symmetry, the most important example of which is rotational symmetry. This more general calculation is important because it has applications to important physical problems like atoms and nuclear shell structure. We will present the calculation for non-Abelian symmetry in a future paper.

An issue that we have largely bypassed in this paper, but hope to address in future publications, is the connection with symmetry-reduced dynamics. Equation (5.1) makes use of the full dynamics of the system in question. In practice, however, if one needed to deal with a system with symmetry, a useful practice would be to use that symmetry to reduce the Hamiltonian. In quantum mechanics this would mean decomposing the Hamiltonian into its irreducible components, corresponding to the irreducible representations of the symmetry group. There is an analogous procedure in classical mechanics whereby one uses the symmetry to achieve a reduction in the number of degrees of freedom. An obvious question is whether one can relate the spectrum of an irreducible component of the Hamiltonian, determined by energy levels of a given symmetry class, to the reduced classical dynamics.

This question has been answered in the affirmative by Robbins [20] for the case of discrete symmetry. He shows that the density of states of an irreducible component of the Hamiltonian is given by a trace formula involving the periodic orbits of the classically reduced system. It seems clear that a similar relationship should exist in the case of continuous symmetries, so that the trace formulas we have derived could be decomposed into individual sums for the density of states of each irreducible component, with each sum involving periodic orbits of the reduced system. Indeed, for axial symmetry this is already known to be the case [6,7]. It needs to be understood in a more general context, however, and is something we hope to report on in the future.

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## APPENDIX A

While manipulating Jacobians in this paper, we use certain tricks repeatedly. It is therefore worthwhile stating them explicitly, as we do in this appendix.

Let $(p,q)$, $(r,s)$, and $(u,v)$ be alternative sets of independent variables ($p,q$, etc., may be multidimensional). We make frequent use of the chain rule

$$\frac{\partial(p,q)}{\partial(u,v)}=\frac{\partial(p,q)}{\partial(r,s)}\frac{\partial(r,s)}{\partial(u,v)} \tag{A1}$$

both to combine Jacobians and also to break up existing Jacobians into Jacobians that depend on more desirable arguments. A less obvious identity that we use is the following:

$$\left|\frac{\partial(u,v)}{\partial(r,v)}\right|=\left|\left[\frac{\partial u}{\partial r}\right]_v\right|, \tag{A2}$$

where the Jacobians are enclosed by bars to emphasize that the determinants are being taken. Here, as in the rest of the paper, a subscript on a Jacobian indicates that the variable is held fixed while derivatives are taken. This identity is found by explicitly writing out $\partial(u,v)/\partial(u,r)$ in components and expanding the determinant by means of Cramer's rule. The first use of (A2) occurs in Eq. (2.15), where it is used to bring $\mathbf{x}'_{\|}$ and $E$ into the argument of the Jacobian there.

## APPENDIX B

In this appendix we will collect together the various structures that arise in the trace formula for systems with symmetry and compare them with their counterparts in the usual trace formula. The major difference is that the trace formula for systems with symmetry involves a sum over $(1+k)$-dimensional families $\Gamma$ of periodic orbits rather than individual orbits. The parametrization of $\Gamma$ with the $1+k$ coordinates $(t,\boldsymbol{\theta})$ contrasts the parametrization of a single orbit with the coordinate $t$. The natural measure of $\Gamma$ is in terms of the volume element $dt\,d\boldsymbol{\theta}$ rather than the measure $dt$ of a single orbit. This manifests itself in the final result in that the period of a primitive orbit $T_0$, appearing in Eq. (1.1), is replaced by $T_0V_0$, where $V_0$ comes from a $\boldsymbol{\theta}$ integral over $\Gamma$.

Surface of section mappings also arise in a different way. In systems with symmetry one can restrict the dynamics to a $(2n-1-k)$-dimensional level surface of $(H,\mathbf{J})$ rather than the $(2n-1)$-dimensional energy shell $H=E$. One then chooses a surface of section to be of codimension $1+k$ in a level surface of $(H,\mathbf{J})$ rather than codimension 1 in a level surface of $H$. The dimension of one of these reduced surfaces of section is then $2(n-1-k)$, as compared to $2(n-1)$ in the case of a system without symmetry. To generate the reduced surface

of section mapping, $(1+k)$ parameters $(t,\boldsymbol{\theta})$ are varied instead of the single parameter $t$. Finally, the surface of section mapping enters into the trace formula through the term $\det(M-I)$, where $M$ is of size $2(n-1-k)$ rather than $2(n-1)$.

Finally, we find that for systems with symmetry, generalized periodic orbits as well as ordinary periodic orbits, are of interest. These arise through the factor $\partial\boldsymbol{\Theta}/\partial\mathbf{J}$. Just as ordinary periodic orbits exist at each value of the energy, with varying period $T$, generalized periodic orbits occur at each value of $(H,\mathbf{J})$, with different values of the generalized period $(T,\boldsymbol{\Theta})$. Collectively, the generalized periodic orbits define a $2(1+k)$-dimensional manifold $\Lambda$ (Appendix D), for which the analog in systems without symmetry is a two-dimensional orbit cylinder. $\Lambda$ is generally transversal to the reduced surface of section in phase space and corresponds to eigenvalue 1 in a linearization of the full-phase-space dynamics (Appendix D).

## APPENDIX C

In this appendix, we will show that the reduced surface of section mapping $\psi\colon \Sigma\to\Sigma$ is symplectic with respect to the symplectic structure induced on $\Sigma$ from full phase space. We consider the symplectic form $\Omega|_\Sigma$ obtained by restricting the full-phase-space symplectic form $\Omega$ to $\Sigma$.

The mapping $\psi$ is symplectic with respect to $\Omega|_\Sigma$ if, for any two vectors $u$ and $v$ tangent to $\Sigma$ at some point $\mathbf{z}$,

$$\Omega(\psi_* u,\psi_* v)=\Omega(u,v)\ , \tag{C1}$$

where $\psi_* u$ denotes the linearized propagation if $u$ by the map $\psi$. To check this condition let us relate the vectors $\psi_* u$ and $\psi_* v$ to the constant-$(t,\boldsymbol{\theta})$ mapping $\phi_{t\theta}\equiv h_\theta\phi_t$ appropriate to the point $\mathbf{z}$, which we know to be symplectic. While $\psi\mathbf{z}=\phi_{t\theta}\mathbf{z}$, a point on $\Sigma$ that is infinitesimally displaced from $\mathbf{z}$ will require propagation by a slightly different $t$ and $\boldsymbol{\theta}$. Let $dt(w)$ and $d\theta_a(w)$ be the additional propagation increments for a point displaced from $\mathbf{z}$ by the vector $w$. Then we find

$$\psi_* w=\phi_{t\theta_*}w+dt(w)X_H+d\theta_a(w)X_{J_a}\ , \tag{C2}$$

where we use the summation convention on the $a$ index, and where $X_H$ and $X_{J_a}$ are the vector fields associated with Hamiltonians $H$ and $J_a$, respectively (see Fig. 5). From this we find that

$$\begin{aligned}\Omega(\psi_* u,\psi_* v)=\Omega(u,v)&+\{J_a,J_b\}d\theta_a(u)d\theta_b(v)\\&+d\theta_a(u)dJ_a(\phi_{t\theta_*}v)\\&-d\theta_a(v)dJ_a(\phi_{t\theta_*}u)\ ,\end{aligned} \tag{C3}$$

where we make use of the fact that $\phi_{t\theta}$ is symplectic, as well as the identities $\Omega(X_F,X_G)=\{F,G\}$ and $\Omega(X_F,w)=dF(w)$ for arbitrary functions $F$ and $G$, and vector $w$. Energy conservation is already taken into account in (C3). Using in addition the fact that $\Sigma$ is at constant $\mathbf{J}$ and $\{J_a,J_b\}=0$, we automatically find that condition (C1) is satisfied and $\psi$ is symplectic, as asserted.

## APPENDIX D

The reduced surface of section map $\psi\colon \Sigma\to\Sigma$ plays an important role in the derivation of the semiclassical trace formula, entering into the final result through the term $\det(M-I)$. As constructed in Sec. III, the map $\psi$ is a very useful conceptual tool in interpreting the trace formula. However, when using the trace formula in practical calculations, it may not always be convenient to compute $\det(M-I)$ through $\psi$ in the manner described in Sec. III. In this appendix we will present a method by which it is possible to extract the necessary information from a linearization of the dynamics on full phase space, eliminating the need for an explicit calculation of $\psi$ in computing the trace formula. While this in itself may not be a compelling reason to use the full-phase-space dynamics—we saw in Sec. IV that $\det(M-I)$ can be found just as easily from a regular surface of section mapping in the symmetry-reduced dynamics—the use of a linearized full-phase-space dynamics has the added advantage that it yields the term $\partial\boldsymbol{\Theta}/\partial\mathbf{J}$ in a very convenient way. We will show that $\partial\boldsymbol{\Theta}/\partial\mathbf{J}$ can be interpreted as a submatrix of the full-phase-space monodromy matrix.

As discussed in Sec. III, the quantity $\det(M-I)$, through which the reduced surface of section enters into the final results of this paper, is an invariant of $\Gamma$. That is, it depends neither on the coordinates used on $\Sigma$ nor on $\Sigma$ itself. Since $\psi$ is a symplectic map (Appendix C) the eigenvalues of $M$ occur in reciprocal pairs $(\lambda,1/\lambda)$, allowing us to write

$$\det(M-I)=\prod_{\substack{\text{reciprocal}\\ \text{pairs}}}(\lambda-1)\left[\frac{1}{\lambda}-1\right]\ . \tag{D1}$$

If $m$ is the linearization of the equal-time mapping $\phi_T$ in the full phase space, evaluated at any point on $\Gamma$, it turns out that these $\lambda$'s are eigenvalues of $m$ also. We can therefore determine $\det(M-I)$ from the appropriate eigenvalues of $m$, eliminating the need for the construction of reduced surface of section mappings. The eigenvalues of $M$ determine $2(n-1-k)$ eigenvalues of $m$. We will show that the remaining $2(k+1)$ eigenvalues of $m$ are equal to 1, that is the eigenvalue 1 occurs with multiplicity $2(k+1)$. Therefore the eigenvalues of $m$ entering into (D1) are precisely those eigenvalues that are not equal to 1.

First we note that the $k+1$ vectors $X_H,X_{J_a}$ are eigenvectors of $m$ with eigenvalue 1. This is obvious since these vectors all point along $\Gamma$ and are therefore carried into themselves under a single iteration of $\phi_T$. The subspace corresponding to eigenvalue 1, $V$ say, includes more than just these vectors, however; it is the tangent space to the $2(k+1)$-dimensional surface $\Lambda$, where $\Lambda$ is a manifold consisting of all generalized periodic orbits near $\Gamma$. We can write $\Lambda=\bigcup_{JH}\Gamma_{JH}$, where each $\Gamma_{JH}$ is the family of generalized periodic orbits at a given value of $\mathbf{J}$ and $H$ (denoted by $\Gamma$ in the particular case of a regular periodic family). Consider any $k+1$ vectors $(e_{J_a},e_H)$ tangent to $\Lambda$ in such a way that,

$$dH(e_H)=1,\quad dJ_a(e_H)=0\ ,$$
$$dH(e_{J_b})=0,\quad dJ_a(e_{J_b})=\delta_{ab}\ . \tag{D2}$$

Each of these vectors points to a particular generalized periodic orbit family $\Gamma_{\mathbf{J}H}$ and therefore evolution under $\phi_T$ brings the tip of each one to within an infinitesimal $(t,\boldsymbol{\theta})$ evolution of itself (see Fig. 5). More precisely,

$$me_H=e_H-\frac{\partial T}{\partial E}X_H-\frac{\partial\Theta_a}{\partial E}X_{J_a}\ ,$$
$$me_{J_b}=e_{J_b}-\frac{\partial T}{\partial J_b}X_H-\frac{\partial\Theta_a}{\partial J_b}X_{J_a}\ , \tag{D3}$$

where $(T,\boldsymbol{\Theta})$ is the generalized period of $\Gamma_{\mathbf{J}H}$. Therefore the action of $m$ on the subspace $V$ is described by the following $2(1+k)\times 2(1+k)$ matrix:

$$m_1=\begin{bmatrix} I-\begin{bmatrix} \frac{\partial T}{\partial E} & \frac{\partial T}{\partial \mathbf{J}} \\ \frac{\partial\boldsymbol{\Theta}}{\partial E} & \frac{\partial\boldsymbol{\Theta}}{\partial \mathbf{J}} \end{bmatrix} \\ 0 \qquad\qquad I \end{bmatrix}, \tag{D4}$$

all of whose eigenvalues are equal to 1. This subspace $V$, spanned by $(X_H,X_{J_a},e_H,e_{J_b})$, is a tangent to $\Lambda$ and in fact we can think of the vectors $(X_H,X_{J_a},e_H,e_{J_b})$ as coordinate basis vectors for coordinates $(t,\boldsymbol{\theta},H,\mathbf{J})$ on $\Lambda$.

The remaining eigenvalues of $m$, which are not equal to 1, define another subspace $W$ that is transverse to $\Lambda$ in phase space. It is easy to see that this subspace is skew-orthogonal to $V$, since these subspaces correspond to different eigenvalues of $m$. In particular, $\Omega(X_H,u)=dH(u)=0$ and $\Omega(X_{J_a},u)=dJ_a(u)=0$ for any vector $u$ in $W$, so $W$ is along constant $H$ and $\mathbf{J}$. The subspace $W$, along with the vectors $(X_H,X_{J_a})$, spans the level surface of $(\mathbf{J},H)$ at $\Gamma$. Under projection onto a reduced surface of section $\Sigma$, the vectors $(X_H,X_{J_a})$ are mapped to a single point in $\Sigma$ and the space $W$ is mapped surjectively onto $\Sigma$, with an eigensubspace of $m$ being mapped onto the eigensubspace of $M$ corresponding to the same eigenvalue. In other words, the linearized dynamics on the reduced surface of section is equivalent to the dynamics of $m$ restricted to $W$.

We have seen that the factor $\det(M-I)$ can be determined from a linearization of the full-phase-space dynamics by picking out the appropriate eigenvalues of $m$. Using (D3) and (D4) we can also use the full-phase-space dynamics to determine $\partial\boldsymbol{\Theta}/\partial\mathbf{J}$, and in a way that would be straightforward to implement in a numerical calculation. We do this by computing $m_1$ of (D4). Given the matrix $m$, it is straightforward to decompose phase space into the eigensubspaces of $m$, giving $V$ and $W$. Corresponding to the subspace $V$, one can then extract from $m$ a $2(1+k)\times 2(1+k)$ matrix that is similar to $m_1$, and in fact this matrix is equal to $m_1$ when computed in the basis $(X_H,x_{J_a},e_H,e_{J_b})$ for $V$. The vectors $X_H$ and $X_{J_a}$ are easily computed from Hamilton's equations and for $e_H$ and $e_{J_b}$ one can take any $1+k$ vectors in $V$ that satisfy the conditions of (D2). In this way $m_1$ is computed from $m$. One can then extract $\partial\boldsymbol{\Theta}/\partial\mathbf{J}$ as a submatrix of $m_1$, as shown in (D4).

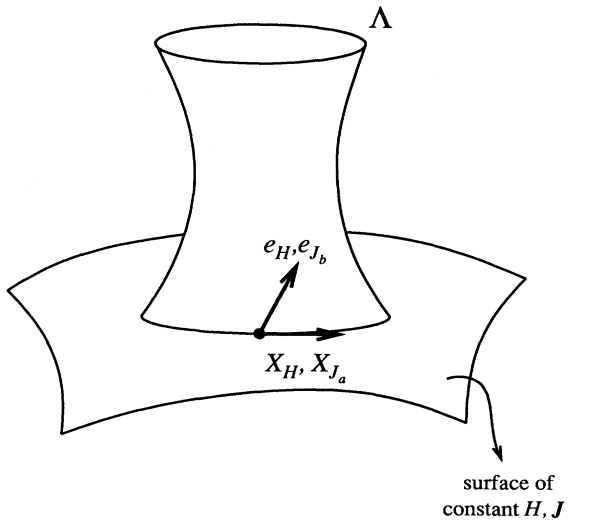


FIG. 5. A highly schematic representation of the dynamics on $\Lambda$, in which many dimensions have been suppressed. The picture is reasonably faithful in the special case $k=0$. Each individual family $\Gamma_{\mathbf{J}H}$ is invariant under $(t,\boldsymbol{\theta})$ evolution, so a point on some $\Gamma_{\mathbf{J}H}$ near $\Gamma$ is mapped to a nearby point on the same $\Gamma_{\mathbf{J}H}$ by the time evolution $\phi_T$, where $T$ is the period of $\Gamma$. The resulting small displacement on $\Gamma_{\mathbf{J}H}$ can be expressed as a linear combination of the vectors $(X_H,X_{J_a})$. In particular, the vectors $(e_H,e_{J_b})$, which point along $\Lambda$, are mapped by $\phi_T$ into vectors that are displaced from the original vectors by linear combinations of $X_H$ and $X_{J_a}$.

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