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Semiclassical trace formulae for systems with non-Abelian symmetry

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Abstract. We derive generalizations of the trace formula of Gutzwiller and Balian and Bloch that are valid in the presence of a non-Abelian continuous symmetry. The usual trace formula must be modified in such cases because periodic orbits occur in continuous families, whereas the usual trace formula requires that the periodic orbits be isolated at a given energy. These calculations extend the results of a previous paper, in which we considered Abelian continuous symmetries. The most important application of the results of this paper is to systems with full three-dimensional rotational symmetry, and we give this case special consideration.

1. Introduction

In a previous publication [1] (hereafter referred to as I), we derived a generalization of the Gutzwiller trace formula [2, 3] that is valid in the case that a continuous Abelian symmetry is present. In this paper we will extend the results to the case of non-Abelian symmetry. The usual trace formula of Gutzwiller does not apply in systems with continuous symmetries, because its derivation includes an assumption that periodic orbits are isolated at a given energy, and because in systems with continuous symmetries, periodic orbits are not isolated. In fact, in the typical case, periodic orbits in a system with a continuous symmetry appear in $(k+1)$-dimensional manifolds, where k is the dimension of the symmetry group.

As shown in I, the appropriate trace formula in systems with continuous Abelian symmetries involves a discrete sum, not over individual periodic orbits, which are no longer countable, but rather over whole manifolds of periodic orbits. In this paper we generalize these results to the case of non-Abelian symmetries, with special attention given to the case of rotational symmetry. Let us summarize briefly the results that apply to the case of Abelian symmetry. The trace formula derived in I for this case has the following form,

$$\rho_{\mathrm{osc}}(E) \approx \frac{1}{\pi\hbar}\frac{1}{(2\pi\hbar)^{k/2}} \sum_{\substack{\text{periodic}\\ \text{orbit}\\ \textit{families}}} \frac{T_0 V_0 \cos\left(\dfrac{S}{\hbar} - \dfrac{\sigma\pi}{2} - \dfrac{k\pi}{4}\right)}{|\partial\Theta/\partial J|^{1/2}|\det(M-I)|^{1/2}} \tag{1.1}$$

where $\rho_{\mathrm{osc}}(E)$ is the oscillating part of the quantum mechanical density of states $\rho(E)$.

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The sum is over continuous families Γ of periodic orbits. The phase contribution $S(E)$ is the action of any one of the periodic orbits in the family and σ is the Maslov index. The k-vector $\boldsymbol{J}$ consists of the k first integrals whose existence is implied by the presence of a k-dimensional symmetry group. Note that the $\boldsymbol{J}$-components are not usually action variables in the sense of integrable systems. These first integrals, along with the Hamiltonian H, allow one to reduce the dynamics to a $(n-1-k)$ degree-of-freedom surface of section mapping, and a linearization of this mapping gives the $(n-1-k)\times(n-1-k)$ reduced surface of section matrix M. The factor T_0V_0 measures the $(1+k)$-volume of a family Γ in terms of a volume element that is obtained in a natural way from a parametrization of Γ by the symmetry group and by time. It is a direct generalization of the factor of T_0—the period of a primitive orbit—that is present in Gutzwiller's formula for isolated orbits and is explained in detail in I. Finally, the term $\partial\boldsymbol{\Theta}/\partial\boldsymbol{J}$ measures the amount by which periodic orbits of the reduced dynamics that are close to Γ fail to be periodic in the full phase space (the components of $\boldsymbol{\Theta}$ are coordinates on the symmetry group and correspond to an additional symmetry transformation that is required to close the orbits in full phase space). This is also explained in detail in I, and its analogue for non-Abelian symmetries will be discussed in this paper.

As we will see in this paper, each of the terms that contribute to (1.1) has a direct generalization to the case in which the symmetry of the system in question is non-Abelian. The non-Abelian nature of the symmetry, however, means that many issues that are trivial in the Abelian case have much more interesting structure when one tries to generalize the calculations. We will investigate those differences in this paper.

In terms of dynamics, a major difference is that the first integrals that are connected with the symmetry will not Poisson commute when the symmetry is non-Abelian. This has many implications, the most important of which arise in the reduction process. ('Reduction' is the process, described by Abraham and Marsden [4], whereby symmetries are used to reduce dynamics to a system with fewer degrees of freedom. It is a generalization of the elimination of ignorable coordinates.) When the first integrals are in involution, reduction to a system with fewer degrees of freedom is straightforward, reducing, essentially, to the elimination of ignorable coordinates. The reduction process is more complicated when the first integrals are not in involution, and cannot be understood entirely in terms of ignoring coordinates. A particular consequence of the symmetry being non-Abelian is that the reduction process does not allow one to reduce the number of degrees of freedom to the same extent as in the Abelian case: when the first integrals are in involution one can eliminate a degree of freedom for every independent first integral, whereas not every first integral allows a reduction of a degree of freedom when the first integrals are not in involution. As a consequence of all this, the reduced surface of section matrix M arises in a somewhat different manner when a non-Abelian symmetry is present and, in particular, will be larger than $(n-1-k)\times(n-1-k)$.

There are also implications for the other contributions to the trace formula when the symmetry is non-Abelian. The nearby periodic orbits of the reduced system are no longer parametrized by the complete set of first integrals $\boldsymbol{J}$, or by a complete set of coordinates $\boldsymbol{\Theta}$ on the symmetry group—a reduced set of variables is required. Therefore $\partial\boldsymbol{\Theta}/\partial\boldsymbol{J}$ needs reinterpretation. In addition, the contribution of the group to the T_0V_0 factor, representing a $(1+k)$-volume of the periodic manifold, involves the invariant Haar measure of the group, which is trivial in the Abelian case. These aspects are discussed in detail in the main text of the paper.

The results presented in this paper, as well as those in I, expand on previous results for systems with continuous symmetry. These previous results include the original papers of Balian and Bloch [3], in which trace formulae were developed for billiard systems with continuous families of periodic orbits under quite general conditions. Also, Strutinskii and Magner [5] have found explicit formulae for specific degenerately integrable systems. These results have applications to nuclear shell structure, where the shell structure of nuclei can be understood as arising from fluctuations in the density of states that arise due to a small number of families of periodic orbits [5-7]. We expect that the results presented in this paper for rotational symmetry will be useful in further understanding calculations of this sort. Berry and Tabor [8] have derived trace formulae for integrable systems. As discussed in I, the results derived there can reproduce the results of Berry and Tabor in a straightforward way. We mention also work in a different context by Chazarain [9] and Duistermaat and Guillemin [10], who develop Gutzwiller-like formulae for wave operators on manifolds in which periodic orbits are allowed to arise in continuous families.

The most important single example of the systems we consider in this paper is that of a system with rotational symmetry. Before considering the case of a completely general symmetry, we will present a specialized calculation for the rotational case in section 3. The case of rotational symmetry has the advantage that many of the group-theoretical aspects of the calculation are intuitively obvious and it is not necessary to invoke the abstract group theory that is needed in the general case. This is part of the reason why we first give the calculation for rotational symmetry before delving into the general case. The general case that we consider in section 4, is that the symmetry group is a k-dimensional Lie group. While we try to keep the calculations self-contained, it is useful, for the purposes of following the calculations in section 4 and several of the appendices, to be familiar with the notation of differential geometry and also with the theory of reduction as described in Abraham and Marsden [4]. On the other hand, the calculations for rotational symmetry, as described in section 3, can be understood without recourse to this theory.

To simplify the presentation, we will make some additional assumptions about the manner in which the symmetry group acts on phase space. The first is that the vector fields on phase space representing the action on phase space of infinitesimal group elements are linearly independent near the periodic orbits. The second is that the Poisson brackets of the associated first integrals obey certain relationships that are connected with the Lie bracket on the Lie algebra of the group. This is the assumption of equivariance. Both of these conditions are explained in more detail in section 4 and hold for typical cases of rotational symmetry. We also assume that the Hamiltonian vector field is linearly independent of the infinitesimal symmetry operations. These conditions are not fundamental in any way but allow a more concise presentation of the basic calculation in section 4. We outline the completely general calculations in the appendices.

2. Summary of previous results

While deriving (1.1) in I, we discussed the derivation of trace formulae under quite general settings. In this section we will recall those results in I that are directly applicable to the case of non-Abelian symmetry. The result of interest is an expression for the density of states as a sum over continuous families of periodic orbits. The contribution

from each family involves an explicit, but non-trivial, integral over that periodic orbit family. The calculations in later sections will be directed at computing this integral.

The derivation of the trace formula proceeds along the following lines. One starts with a semiclassical approximation for the energy-dependent Green function in terms of classical trajectories. This may be in a purely position-dependent representation or it may be in a mixed position-momentum representation—either one might be appropriate under different circumstances. One then uses this approximation to compute the trace $g(E)$ of the Green function by means of the stationary phase approximation. The stationary phase approximation receives contributions from those trajectories that are periodic, so that one ends up with an approximation for $g(E)$ in terms of periodic orbits. From the relationship $\rho(E) = -(1/\pi)\,\mathrm{Im}\, g(E)$ we then find that the density of states $\rho(E)$ is also determined by a sum over periodic orbits.

In I we used a mixed representation Green function $G(\boldsymbol{p}, \boldsymbol{x}', E) = \langle \boldsymbol{p}|G(E)|\boldsymbol{x}'\rangle$ (where $G(E)$ is the abstract operator) to compute a trace formula for systems with symmetry. This representation of the Green function can be approximated in terms of a sum over trajectories at energy E that begin at position $\boldsymbol{x}'$ and end with momentum $\boldsymbol{p}$ [1]. The trace $g(E)$ is obtained from $G(\boldsymbol{p}, \boldsymbol{x}', E)$ according to,

$$g(E) = \frac{1}{(2\pi\hbar)^{n/2}} \int \mathrm{d}\boldsymbol{x}' \int \mathrm{d}\boldsymbol{p}\, \exp(\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}'/\hbar) G(\boldsymbol{p}, \boldsymbol{x}', E). \tag{2.1}$$

This is a $2n$-dimensional integral (where n is the number of degrees of freedom) over the collective variable $\bar{z}$, which is defined by $\bar{z} = (\boldsymbol{x}', \boldsymbol{p})$. In computing the integral in (2.1) by the stationary phase approximation, it is found that the stationary phase contributions come from points $\bar{z}$ that correspond to periodic orbits. If there is a k-dimensional symmetry present, the periodic orbits will arise in $(1+k)$-dimensional manifolds (1 dimension for time and k dimensions for the symmetry), and we must perform a degenerate stationary phase calculation to compute $g(E)$. Loosely speaking, we find that the integration across the periodic orbit manifold can be computed using the regular stationary phase approximation, leaving a $(1+k)$-dimensional integral along the periodic orbit manifold which does not have a rapidly varying phase and which must therefore be computed exactly.

The details of this calculation depend to a large extent on whether $1+k \leqslant n$ or $1+k > n$. In I we considered the case $1+k \leqslant n$ and we will concentrate on that case here also. If all the constants of the motion are in involution, which is the case considered in I, this necessarily holds. This condition also holds for the three-body problem (e.g. the helium atom), where $n=6$ after translational symmetry is removed and $k=3$ (corresponding to rotational symmetry). There are also interesting cases, however, for which $1+k > n$—for example spherical symmetry in three degrees of freedom, where $1+k=4$ and $n=3$. Therefore this case should also be considered in general. While the details of the calculation in this latter case are very different to those for $1+k \leqslant n$, the final results have exactly the same structure. For this reason, we will not present much of this calculation, but rather will give a brief summary in appendix A.

When $1+k \leqslant n$, we can split $\bar{z}$ into two sets of components, $\boldsymbol{x}'_{\parallel}$ and $(\boldsymbol{x}'_{\perp}, \boldsymbol{p})$, where $\boldsymbol{x}_{\parallel}$ are $1+k$ configuration space coordinates whose coordinate axes we can take to be parallel to the periodic orbit family in configuration space. The remaining $(n-1-k)$ configuration space coordinates are denoted by $\boldsymbol{x}_{\perp}$. The integral over the $(\boldsymbol{x}'_{\perp}, \boldsymbol{p})$ coordinates in (2.1) can then be computed by means of the regular stationary phase approximation, leaving a $(1+k)$-dimensional integral over the $\boldsymbol{x}_{\parallel}$ coordinates. If we

think of $x_\parallel$ as local coordinates on the periodic orbit manifold, this remaining integral can be interpreted as a volume integral over the periodic orbit manifold itself. In this way, $g(E)$ is determined as a sum over periodic orbit manifolds, where each contribution is given by a $(1+k)$-dimensional integral over a periodic orbit manifold.

In I we explicitly performed the calculation outlined above and obtained the following result,

$$g(E) \approx \frac{1}{i\hbar} \frac{1}{(2\pi i\hbar)^{k/2}} \sum_\Gamma A(\Gamma) \exp\left(\frac{i}{\hbar} S(E) - i\sigma\pi/2\right) \tag{2.2}$$

where,

$$A(\Gamma) = \int_\Gamma dx_\parallel \left| \left(\frac{\partial(z_\perp - z'_\perp, x_\parallel, E)}{\partial(z'_\perp, p'_\parallel, t)} \right)_{x'_\parallel} \right|^{-1/2}. \tag{2.3}$$

The sum in (2.2) is over periodic orbit manifolds Γ at energy E. Each periodic orbit manifold Γ contributes an oscillatory term whose phase is determined by the Maslov index σ and the action $S(E)$ of a periodic orbit in Γ. The amplitude $A(\Gamma)$ of each contribution is given by an integral over Γ, given by (2.3), whose integrand depends on certain dynamical properties of the orbit. We denote by $p_\parallel$ and $p_\perp$, the momenta conjugate to $x_\parallel$ and $x_\perp$ respectively, and we let $z_\parallel = (x_\parallel, p_\parallel)$ and $z_\perp = (x_\perp, p_\perp)$. Primed quantities refer to the initial point of a trajectory that starts near Γ and unprimed quantities refer to the final point of the trajectory.

The Jacobian in (2.3) warrants more discussion. First of all, the subscript $x'_\parallel$ means that the variable $x'_\parallel$ is held fixed while all derivatives are taken. The Jacobian is then one that relates two alternative sets of $n+1$ variables; (z', t) in the denominator and $(z_\perp - z'_\perp, x_\parallel, x'_\parallel, E)$ in the numerator. It is possible to regard each of these sets of variables as providing a parametrization of the set of all trajectories in phase space, where z' is the initial point, z is the final point, t is the time of the trajectory, and E is its energy. An equivalent point of view is that each set of variables forms a set of coordinates for the extended phase space $\mathscr{P} = P \times \mathbb{R}$, where P is phase space and $\mathbb{R}$ represents a time axis. There is a natural coordinate system (z, t) on $\mathscr{P}$ defined in the obvious way. We can also consider coordinates (z', t), where z' is defined through $z = \phi_t z'$, in which ϕ_t is the time-t mapping on phase space. One can similarly define coordinates $(z_\perp - z'_\perp, x_\parallel, x'_\parallel, E)$ by mixing z and z' components. With these interpretations, the meaning of (2.3) is clear.

The calculations of this paper from here on will be aimed at computing the integral that is present in (2.3) in terms of dynamical properties of the periodic orbit manifold that are more easily determined in practice. We first consider rotational symmetry in section 3, before considering more general cases in section 4.

3. Case of rotational symmetry

In this section we will derive a trace formula, analogous to (1.1), that is valid for systems exhibiting rotational symmetry. Technically, we assume that H is invariant under some action of the group SO(3) on phase space by symplectic transformations. While the paradigm for this kind of system is provided by systems of interacting particles in 3D space, we will try not to make assumptions as to the precise nature of the action of SO(3) on phase space. We will assume however, that the action of SO(3) on phase space is 'locally free'. That is, the subgroup which leaves a typical point in

phase space invariant is discrete, so that when the whole group acts on a typical point, a 3D surface is swept out. We also assume that the flow of H is in turn locally independent of the symmetry, so that a 4D surface is obtained when both the flow and the symmetry group act on a point. Finally, the calculations presented are for spinless particles.

As a consequence of rotational symmetry, we find, in addition to H, three independent constants of the motion, namely the three components of angular momentum $\boldsymbol{J}$. For systems of interacting particles in 3-space, $\boldsymbol{J}$ is the total orbital angular momentum. For more general actions of SO(3), the three components of $\boldsymbol{J}$ are defined as being those Hamiltonians that generate infinitesimal rotations about three orthogonal directions. As far as deriving a trace formula is concerned, an important difference between rotational symmetry and the symmetries considered in I is that rotations do not conserve $\boldsymbol{J}$. We will assume that $\boldsymbol{J}$ transforms under rotation of phase space according to,

$$\boldsymbol{J}(Rz) = R\boldsymbol{J}(z). \tag{3.1}$$

(While this is true for every system of physical interest, such as interacting particles in 3-space, it may not hold for exotic group actions and must therefore be made an assumption. We stress the condition here because the analogous condition for the general calculation in the next section is not as obvious.) Actions that satisfy (3.1) are called equivariant.

In the presence of rotational symmetry, a given periodic orbit γ_0 will generally be imbedded in a 3-parameter family of orbits, parametrized by rotations R according to $\gamma_R = R\gamma_0$. We will assume that rotational symmetry is the only (continuous) symmetry present, so that this 3-parameter family enumerates all of the periodic orbits that are continuously related to γ_0. We can then parametrize the corresponding periodic orbit manifold Γ by (t, R), where t is a time coordinate along periodic orbits and R is a rotation. In addition to purely rotational symmetry, there may also be discrete symmetries. For example the system might typically be symmetric under spatial inversions, so that O(3) is a symmetry group. The effect of these extra symmetries will be to produce a discrete set of families, Γ_i say, such that the orbits within a given family are related to each other through pure rotations, and different families are related to each other through discrete symmetry operations. In the calculations that follow we will concentrate on the contribution of an individual family, and therefore we will refer only to the SO(3) component of the symmetry group. To account for the remaining symmetries, we merely sum discretely over the families Γ_i. From now on we suppress the label i on Γ_i.

The parametrization (t, R) above allows us to define a natural measure $\mathrm{d}t\,\mathrm{d}\mu(R)$ on Γ, where $\mathrm{d}\mu(R)$ is the invariant measure for SO(3) [11]. The measure $\mathrm{d}\mu(R)$ is that measure, unique up to a constant factor, that is invariant under left and right translation on SO(3). (While for general groups it is necessary to make a distinction between left- and right-invariant measures, they coincide for compact groups like SO(3), so the distinction need not be made.) We will find that the volume element defined by the integrand of (2.3) is proportional to $\mathrm{d}t\,\mathrm{d}\mu(R)$ on Γ. The integral in (2.3) then reduces to a normalization of $\mathrm{d}t\,\mathrm{d}\mu(R)$ over Γ, which gives a contribution to the trace formula that is analogous to the $T_0 V_0$ factor in (1.1).

All of this is analogous to the use in I of coordinates $(t, \boldsymbol{\theta})$ to parametrize Γ. These coordinates were evolution parameters for the Hamiltonian flows of the first integrals $(H, \boldsymbol{J})$ on Γ. We can make this analogy more direct by introducing a similar set of coordinates $(t, \boldsymbol{\theta})$ in the rotational case, where the $\boldsymbol{\theta}$-components are now evolution

parameters for the components of the angular momentum vector J. The θ coordinates can be physically interpreted as angles of rotation about the corresponding axes in 3-space. Care must be taken when using these coordinates for rotational symmetry because rotations about different axes do not commute. In order to define the coordinates globally one should fix an ordering for the axes of rotation. We will avoid this issue by considering only infinitesimal rotations, for which any two rotations commute to first order in θ. These coordinates are really useful only near $\theta = 0$, and for this reason we will consider such a set of coordinates to be constructed about every periodic orbit γ in Γ. These local coordinates define a volume element $dt\, d\theta$ on Γ, a direct generalization of one constructed in I. We will show in appendix B, where we consider general symmetries, that $dt\, d\theta$ is proportional to $dt\, d\mu(R)$. In fact, we can choose the normalization of $d\mu(R)$ so that $dt\, d\theta = dt\, d\mu(R)$.

We now proceed to simplify (2.3). The overall structure of the calculations is similar to those in I, and we will dwell only on those parts that are different. First we introduce dynamics on an extended phase space $\tilde{\mathcal{P}} = P \times \mathbb{R} \times SO(3)$, where P is phase space and $\mathbb{R}$ corresponds to time. $\tilde{\mathcal{P}}$ generalizes the extended phase space $\mathcal{P}$, described in section 2, to include rotations as well as time evolution. Dynamics on $\tilde{\mathcal{P}}$ is given by $(z', t', R') \to (z = R\phi_t z', t + t', RR')$ in a 'generalized time' (t, R), where we usually take $t' = 0$ and $R' = I$. We can now reinterpret the Jacobian in (2.3) as a Jacobian on $\tilde{\mathcal{P}}$, in which we fix $\theta = 0$. Here we regard θ as local coordinates on SO(3), parametrizing rotations that are infinitesimally close to the identity. We write,

$$\left(\frac{\partial(z_\perp - z'_\perp, x_\parallel, E)}{\partial(z'_\perp, p'_\parallel, t)}\right)_{x'_\parallel} = \frac{\partial(z_\perp - z'_\perp, x'_\parallel, x_\parallel, E, \theta)}{\partial(z'_\perp, z'_\parallel, t, \theta)}. \tag{3.2}$$

Following similar calculations in I, we use the chain rule to break up this Jacobian as follows,

$$\frac{\partial(z_\perp - z'_\perp, x'_\parallel, x_\parallel, E, \theta)}{\partial(z'_\perp, z'_\parallel, t, \theta)} = \left(\frac{\partial(z_\perp - z'_\perp, \theta)}{\partial(z'_\perp, J')}\right)_{x'_\parallel, x_\parallel, E} \left(\frac{\partial(x_\parallel, E, J')}{\partial(p'_\parallel, t, \theta)}\right)_{z'_\perp, x'_\parallel} \tag{3.3}$$

where J' is the initial value of the angular momentum. This step has introduced derivatives in which θ is allowed to vary, so from here on infinitesimal rotations will be included in the trajectories. Unlike the case of Abelian symmetry considered in I, the first integrals J can vary over these small rotations, so it is important to distinguish between the initial value J' and the final value J of the angular momentum.

Also following calculations that are similar to those in I, we can combine the second Jacobian of (3.3) with the volume element $dx_\parallel$ to get the natural measure for Γ as follows,

$$dx_\parallel \left| \left(\frac{\partial(x_\parallel, E, J')}{\partial(p'_\parallel, t, \theta)}\right)_{z'_\perp, x'_\parallel} \right|^{-1/2} = dt\, d\theta = dt\, d\mu(R). \tag{3.4}$$

The steps involved in showing this are essentially identical to those of the analogous calculation in I, so we do not show them here. We just remark that the calculation proceeds by breaking up the Jacobian of (3.4) into two further Jacobians by means of the chain rule. Each of these is the determinant of a $(1+k)\times(1+k)$ matrix, whose columns consist of $x_\parallel$-velocities under the Hamiltonian flows of the functions (H, J). The $1+k$ functions (H, J) label the columns and the $1+k$ components of $x_\parallel$ label the rows. Also, one of the Jacobians is evaluated at the initial point of a trajectory and the other is evaluated at the final point—of course these coincide when evaluated on a periodic orbit. Equation (3.4) then follows from noting that the Hamiltonian vector fields of (H, J) are coordinate basis vectors for the local coordinates (t, θ) on Γ.

The calculations so far allow us to write,

$$A(\Gamma)=\int_{\Gamma} \mathrm{d}t\,\mathrm{d}\boldsymbol{\theta}\left|\left(\frac{\partial(\boldsymbol{z}_{\perp}-\boldsymbol{z}'_{\perp},\,\boldsymbol{\theta})}{\partial(\boldsymbol{z}'_{\perp},\,\boldsymbol{J}')}\right)_{x'_{\parallel},x_{\parallel},E}\right|^{-1/2}. \tag{3.5}$$

We will now work on interpreting the remaining Jacobian in terms of surface of section dynamics. Until now, the calculations have been very similar to those in I. From here on, however, there will be distinct structural differences, reflecting the fact that the reduction process is more complicated for non-Abelian symmetries.

We now describe reduced surface of section mappings that are constructed with the aid of rotational symmetry. First we recall that $\boldsymbol{J}$ is not invariant under the dynamics of $\tilde{\mathscr{P}}$, in which rotations are included. Only the magnitude J of $\boldsymbol{J}$ is invariant. The direction $\hat{\boldsymbol{J}}$ can be mapped into any other direction with an appropriate rotation. We will therefore choose our surface of section, Σ say, to lie in the $(2n-2)$-dimensional invariant surface $\{z|H, J=\text{constant}\}$, where we now focus our attention on phase space P rather than generalized extended phase space $\tilde{\mathscr{P}}$. More specifically, we let Σ be any surface which has codimension 4 within the level surface $\{z|H, J=\text{constant}\}$. The only additional condition is that the four independent vector fields generated by time-evolution and rotations be transverse to Σ. With these conditions, we find that Σ intersects the 4D manifold Γ at isolated points. We will only be interested in surface of section dynamics that takes place near Γ.

To define a surface of section mapping $\psi:\Sigma\to\Sigma$, we first start a trajectory on Σ near Γ, and follow it around Γ under the Hamiltonian flow of H. We then adjust the 4 parameters of generalized time (t, R) to get the trajectory back onto Σ, thereby completing the mapping ψ. Since Σ is even dimensional (its dimension is $2(n-3)$), we can make it into a symplectic manifold in a natural way by restricting the full phase space symplectic form Ω to it. In contrast to the analogous mappings constructed for Abelian symmetries in I however, we find that ψ is not generally symplectic with respect to this symplectic structure. For that to be the case Σ must be chosen so that $\boldsymbol{J}$ is constant on Σ. We will not assume that this is the case. There does exist a symplectic form for Σ in the general case however, with respect to which ψ is symplectic. This is discussed in appendix C.

Notice that while the symmetry group SO(3) is three-dimensional, so that (including H) there are $3+1=4$ independent first integrals, in constructing surfaces of section as above we have reduced the number of degrees of freedom by just $2+1=3$. (In contrast, we saw in I that Abelian symmetries facilitated a reduction of one in the number of degrees of freedom for every independent constant of the motion.) This inhibited reduction is not a result of inefficiency in the construction of Σ, but rather is an intrinsic limitation of the dynamics. Provided the only symmetry present is rotational, we expect that the map ψ is completely generic, exhibiting no further symmetries or invariants. In particular for example, the fixed points of ψ will be isolated in Σ and none of the eigenvalues of M, the linearization of ψ at a fixed point, will equal 1. Therefore $\det(M-I)$ will be non-zero and can contribute to the trace formula in a similar manner to (1.1). Let us proceed to connect (3.5) with this surface of section mapping.

The derivatives in the remaining Jacobian of (3.5) are all taken at constant $(\boldsymbol{x}_{\parallel}, \boldsymbol{x}'_{\parallel}, E)$. We can incorporate this condition into the dynamics by making use of a particular family of surfaces of section, $\Sigma_J=\{z|H, J, \boldsymbol{x}_{\parallel}=\text{constant}\}$, parametrized by J. Useful coordinates for Σ_J are $(\boldsymbol{z}_{\perp}, \hat{\boldsymbol{J}})$. The corresponding surface of section mapping is denoted by ψ_J. The periodic orbit Γ contributing to the trace formula will occur at

a particular value of H and J. In what follows we will always be concerned with surface of section dynamics at the same value of energy $H = E$, but we will want to consider dynamics for values of J that are slightly different from that of Γ. For this reason we suppress the energy-dependence in the notation Σ_J and ψ_J. We denote by Σ the particular Σ_J lying in the same constant J surface as Γ. If we let $z = \psi_J z'$, for any z' in any Σ_J, we find that the restrictions that $(x_\parallel, x'_\parallel, E)$ are held fixed are automatically obeyed. The vector $\boldsymbol{\theta}$ then represents the rotation that is necessary to bring the trajectory of z' back to Σ_J. If $\boldsymbol{\theta}_\parallel$ and $\boldsymbol{\theta}_\perp$ are the components of $\boldsymbol{\theta}$ parallel to $\boldsymbol{J}$ and perpendicular to $\boldsymbol{J}$, respectively, we have,

$$\begin{aligned}\frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta})}{\partial(z'_\perp, \boldsymbol{J}')} &= \frac{\partial(\hat{\boldsymbol{J}}', J')}{\partial(\boldsymbol{J}')} \frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta}_\perp, \boldsymbol{\theta}_\parallel)}{\partial(z'_\perp, \hat{\boldsymbol{J}}', J')} \\ &= \frac{1}{J'^2} \frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta}_\perp, \boldsymbol{\theta}_\parallel)}{\partial(z_\perp - z'_\perp, \boldsymbol{\theta}_\perp, J')} \frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta}_\perp, J')}{\partial(z'_\perp, \hat{\boldsymbol{J}}', J')} \\ &= \frac{1}{J^2} \left(\frac{\partial \boldsymbol{\theta}_\parallel}{\partial J}\right)_{z_\perp - z'_\perp, \boldsymbol{\theta}_\perp} \left(\frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta}_\perp)}{\partial(z'_\perp, \hat{\boldsymbol{J}}')}\right)_J \end{aligned} \tag{3.6}$$

where we have used $J = J'$. In the Jacobians above, we let $\hat{\boldsymbol{J}}$ represent any two coordinates labelling the direction of $\boldsymbol{J}$, defined in such a way that their Jacobian with respect to solid angle is unity.

It turns out that the second Jacobian in the final line above reduces to a term $\det(M - I)$, corresponding to the reduced surface of section mapping. To see this we first note that, to first order in $\boldsymbol{\theta}$, the reduced surface of section mapping rotates $\boldsymbol{J}$ on the sphere $J =$ constant as follows,

$$\hat{\boldsymbol{J}} \approx \hat{\boldsymbol{J}}' + \boldsymbol{\theta} \times \hat{\boldsymbol{J}}' = \hat{\boldsymbol{J}}' + \boldsymbol{\theta}_\perp \times \hat{\boldsymbol{J}}'. \tag{3.7}$$

We can invert this to express $\boldsymbol{\theta}_\perp$ in a one-to-one relationship with $\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}'$ as follows,

$$\boldsymbol{\theta}_\perp \approx \hat{\boldsymbol{J}}' \times (\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}') \tag{3.8}$$

as illustrated in figure 1. Since $\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}'$ is approximately perpendicular to $\hat{\boldsymbol{J}}'$, the transformation $\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}' \to \boldsymbol{\theta}_\perp$ is just a rigid rotation of $\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}'$ by 90° and is therefore area preserving on the sphere $J =$ constant. That is,

$$\left.\frac{\partial(\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}')}{\partial \boldsymbol{\theta}_\perp}\right|_{\boldsymbol{\theta}_\perp = 0} = 1. \tag{3.9}$$

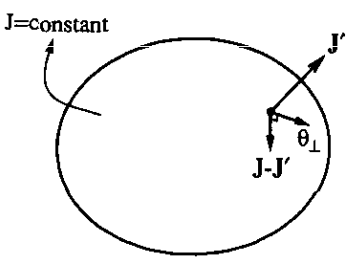

Figure 1. $\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}'$ and $\boldsymbol{\theta}_\perp$ provide alternative parametrizations of the sphere $J =$ constant near $\hat{\boldsymbol{J}}'$. They are related to each other by a rigid rotation of 90°, which is area preserving on the sphere. For this reason the Jacobian relating the corresponding change of variables is equal to 1.

We can therefore write,

$$\frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta}_\perp)}{\partial(z'_\perp, \hat{\boldsymbol{J}}')} = \frac{\partial(z_\perp - z'_\perp, \hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}')}{\partial(z'_\perp, \hat{\boldsymbol{J}}')}$$
$$= \det(M - 1) \tag{3.10}$$

where the last identity follows from using coordinates $(z_\perp, \hat{\boldsymbol{J}})$ on the surface of section Σ. As before, M is the linearization of ψ. The quantity $\det(M - I)$ is an invariant of Γ: it is independent of the coordinates used on Σ and also of the choice of Σ itself. This was discussed in I for the reduced surface of section mappings considered there and the same arguments apply here.

We next consider the factor $(\partial \boldsymbol{\theta}_\parallel / \partial J)_{z_\perp - z'_\perp, \boldsymbol{\theta}_\perp}$ in (3.6). In light of (3.8), we see that keeping $\boldsymbol{\theta}_\perp$ fixed at zero in this derivative is equivalent to fixing $\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}' = 0$, therefore,

$$\left(\frac{\partial \boldsymbol{\theta}_\parallel}{\partial J}\right)_{z_\perp - z'_\perp, \boldsymbol{\theta}_\perp} = \left(\frac{\partial \boldsymbol{\theta}_\parallel}{\partial J}\right)_{z_\perp - z'_\perp, \hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}'} = \frac{\partial \Theta_\parallel}{\partial J} \tag{3.11}$$

where $\Theta_\parallel(J)$ is the rotational component of the generalized period of the generalized periodic orbit at J. We explain this in more detail as follows. We can identify the fixed points of the maps ψ_J with what we call 'generalized periodic orbits'. These are orbits that close in phase space after time evolution and a rotation. Just like ordinary periodic orbits, the generalized periodic orbits arise in 3-parameter families, and there is a one-to-one correspondence between one of these families and a fixed point of the map ψ_J. Because the fixed points are isolated in each Σ_J, there is precisely one generalized periodic orbit family near Γ for each value J of the magnitude of the angular momentum, and we denote this family by Γ_J. Each periodic orbit family will have a generalized period $(T, \Theta_\parallel)$, *where* $\Theta_\parallel$ *is the angle of rotation about the angular momentum* vector that is necessary to close the orbit. The rotation must be about $\boldsymbol{J}$ if we are to have $\boldsymbol{J}$ return to its initial value. It is not difficult to see that $\Theta_\parallel$ is constant on each Γ_J, so $\partial \Theta_\parallel / \partial J$ is well defined. If we note that, fixing $z_\perp - z'_\perp$ and $\hat{\boldsymbol{J}} - \hat{\boldsymbol{J}}'$ at zero defines a fixed point of the map ψ_J, (3.11) follows immediately.

We can collect the preceding calculations in the following expression for the amplitude $A(\Gamma)$,

$$A(\Gamma) = J |\det(M - I)|^{-1/2} \left| \frac{\partial \Theta_\parallel}{\partial J} \right|^{-1/2} \int_\Gamma \mathrm{d}t \, \mathrm{d}\mu(R). \tag{3.12}$$

The next step is to integrate $\mathrm{d}t \, \mathrm{d}\mu(R)$ over Γ. Just like in Gutzwiller's formula for isolated orbits, the time integral gives T_0, the period of the primitive orbit. For the remaining integral it is useful to note the following normalization of $\mathrm{d}\mu(R)$ over SO(3) [11],

$$\int_{\mathrm{SO}(3)} \mathrm{d}\mu(R) = 8\pi^2. \tag{3.13}$$

If there is a one-to-one correspondence between rotations R and periodic orbits γ_R the integral of $\mathrm{d}\mu(R)$ over Γ is given by (3.13). More generally however, there will be a discrete subgroup $I(\gamma_0)$ of SO(3) whose rotations will carry a given periodic orbit γ_0 into itself. In this case (3.13) overcounts by a factor of N_I, the number of elements in $I(\gamma_0)$. Therefore,

$$\int_\Gamma \mathrm{d}t \, \mathrm{d}\mu(R) = T_0 \frac{8\pi^2}{N_I}. \tag{3.14}$$

We can finally write the trace formula for rotationally symmetric systems as follows

$$g(E)\approx\frac{1}{i\hbar}\frac{1}{(2\pi i\hbar)^{3/2}}\sum_{\Gamma}\frac{JT_0\dfrac{8\pi^2}{N_I}\exp\left(\dfrac{i}{\hbar}S(E)-i\sigma\pi/2\right)}{|\partial\Theta_{\|}/\partial J|^{1/2}|\det(M-I)|^{1/2}} \tag{3.15}$$

which is similar in structure to (1.1). Again we point out that the various quantities contributing to this trace formula are intrinsic, coordinate-free properties of the periodic orbit families, just as in Gutzwiller's formula and the trace formula of (1.1) for Abelian symmetries. In addition, notice that, while we have assumed $n\geq 4$ in this section, the various quantities arising in (3.15) make sense even when $n=3$. This suggests that (3.15) is generally valid. As discussed in appendix A, this is indeed true.

4. Case of general non-Abelian symmetry

The calculations of the previous section can be generalized in a straightforward way to systems with more general non-Abelian symmetries. In this section we assume that H is invariant under an action of some k-dimensional Lie group G on phase space by symplectic transformations. We will further assume, as we did for rotational symmetry, that the action of G on phase space is locally free and that the flow of H is in turn locally independent of the action of G. This will ensure the existence of k independent first integrals J, whose Hamiltonian flows generate G. The case where the action of the group is degenerate is considered in appendix D.

The main difference between the calculations for SO(3) and those for more general groups is that much of the group structure of SO(3) is easily interpreted in terms of simple 3D geometry and can therefore be dealt with without explicit reference to group theory. In contrast, the calculations for general groups make explicit use of the group structure. Before delving into the calculation of the trace formula in section 4.2, we summarize briefly in section 4.1 the group-theoretical constructs that we will use. The main purpose is to establish notation and to collect together the various facts that will be used and not to provide a complete description. It is probably necessary, on the part of the reader, to have some prior familiarity with the general theory (concerning coadjoint orbits, momentum maps, etc) for a complete understanding of the calculations. For more detailed explanations of the group theory, with explicit reference to dynamical applications, we refer the reader to Abraham and Marsden [4]. See also Arnol'd [12].

4.1. Group-theoretical preliminaries

We denote by $\mathcal{G}$ the Lie algebra of G, which is the tangent space to G at the identity. We will make frequent use of the exponential map, which takes a Lie algebra element ξ into a group element $\exp(\xi)$, defined as follows. Corresponding to the Lie algebra element ξ, we consider the left-invariant vector field $X_\xi(g)=g\xi$ on G, obtained by left-translating ξ from the identity to g. The integral curve of X_ξ emerging from the identity at $t=0$ is then $\exp(t\xi)$ [4]. We can use the exponential map to define the so-called adjoint representation of G on $\mathcal{G}$. This is defined as the infinitesimal version of the conjugation operation $h\to ghg^{-1}$ as follows,

$$\mathrm{Ad}_g\xi=\frac{d}{dt}\,g\cdot\exp(t\xi)\cdot g^{-1}\Big|_{t=0}. \tag{4.1}$$

It is easy to check that this linear map from $\mathcal{G}$ into itself is indeed a representation of G. It is also useful to let g become infinitesimal in (4.1), leading us to define,

$$\mathrm{ad}_\eta \xi = \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Ad}_{\exp(t\eta)} \xi \Big|_{t=0} \tag{4.2}$$

which is linear in both ξ and η and which can be shown [4] to be related to the Lie bracket on $\mathcal{G}$ according to $\mathrm{ad}_\eta \xi = [\eta, \xi]$.

An important object as far as dynamics is concerned is $\mathcal{G}^*$, the dual space of $\mathcal{G}$. It is the space of all linear functionals on $\mathcal{G}$. We will denote the natural pairing between elements ω of $\mathcal{G}^*$ and elements ξ of $\mathcal{G}$ by either $\omega(\xi)$ or $\langle \omega, \xi \rangle$. The coadjoint representation, $g \to \mathrm{Ad}^*_{g^{-1}}$, of G on $\mathcal{G}^*$ is defined by,

$$\langle \mathrm{Ad}^*_{g^{-1}} \omega, \xi \rangle = \langle \omega, \mathrm{Ad}_{g^{-1}} \xi \rangle \tag{4.3}$$

and its infinitesimal version is

$$\mathrm{ad}^*_\xi = \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Ad}^*_{\exp(-t\xi)} \Big|_{t=0} \tag{4.4}$$

which is connected to the Lie bracket on $\mathcal{G}$ according to $\langle \mathrm{ad}^*_\eta \omega, \xi \rangle = -\langle \omega, [\eta, \xi] \rangle$. The adjoint and coadjoint actions are the natural actions of G on $\mathcal{G}$ and $\mathcal{G}^*$ respectively, and will therefore arise frequently. For this reason we will adopt the simpler notation, $\mathrm{Ad}_g \xi = g \cdot \xi$ and $\mathrm{Ad}^*_{g^{-1}} \omega = g \cdot \omega$, where there is no risk of confusion.

The dual space $\mathcal{G}^*$ is important for dynamics because the collection of first integrals $\boldsymbol{J}$ can naturally be thought of as a vector in $\mathcal{G}^*$. More precisely, we define the so-called momentum map $\boldsymbol{J}: P \to \mathcal{G}^*$ according to

$$\langle \boldsymbol{J}(z), \xi \rangle = J_\xi(z) \tag{4.5}$$

where $J_\xi(z)$, when regarded as a Hamiltonian function on P, generates as its Hamiltonian vector field the infinitesimal generator on P of the Lie algebra element ξ. This construction is described fully in Abraham and Marsden [4]. Because H is G-invariant, we find that H is conserved under the flow of J_ξ, so that $\{H, J_\xi\} = 0$, which in turn implies that J_ξ is conserved under the flow of H. Therefore the k-vector $\boldsymbol{J}(z)$, living in $\mathcal{G}^*$, is invariant under the flow of H, giving k independent first integrals as asserted.

While $\boldsymbol{J}$ is invariant under the flow of H, it is not in general invariant under the action of G on phase space. This defines an action of G on $\mathcal{G}^*$ according to, $\boldsymbol{J}(z) \to \boldsymbol{J}(g \cdot z)$. We have already seen that there is an intrinsic action of G on $\mathcal{G}^*$, which is purely group-theoretical, namely the coadjoint action of (4.3). For convenience, we make the assumption that these actions coincide, that is,

$$\boldsymbol{J}(g \cdot z) = g \cdot \boldsymbol{J}(z). \tag{4.6}$$

Group actions satisfying this condition are called equivariant. In the special case of rotational symmetry the equivariance condition reduces to (3.1) while for Abelian symmetry it is equivalent to the assumption that the first integrals Poisson commute. This assumption is not strictly necessary; if a non-equivariant action arises in practice our calculations still carry through with minor modifications if one lets $g \cdot \boldsymbol{J}$ represent the dynamical action rather than the coadjoint action. We give a brief outline of the more general calculation in appendix E.

A simple example of a classical system with non-equivariant symmetry is provided by the case in which H does not depend on the coordinates (q_n, p_n). The symmetry group consists of translations in the (q_n, p_n)-plane and is Abelian. Consequently, each

coadjoint operator $\mathrm{Ad}^*_{g^{-1}}$ is just the identity map. The Hamiltonian generators for translation along the q_n and p_n axes are, respectively, p_n and $-q_n$. Therefore the momentum map is $J(z) = (p_n, -q_n)$. Notice that translations in the (q_n, p_n)-plane do not leave $J(z)$ invariant whereas $\mathrm{Ad}^*_{g^{-1}}$ does. Therefore (4.6) is violated. It might be objected that this is a silly example because one would not consider the nth degree of freedom to begin with in a case like this. However, this kind of symmetry can arise as a result of a change of coordinates, in such a way that the symmetry is not so trivial beforehand. For example, a charged particle in a uniform magnetic field has translational symmetry. In the so-called called guiding centre coordinates [13] for the problem, there are a pair of canonically conjugate coordinates (X, Y) representing the centre of the circle of gyration. Translational symmetry of the system in the plane perpendicular to the magnetic field manifests itself in the independence of the Hamiltonian of the coordinates (X, Y), and so is an example of non-equivariant symmetry.

Let us now concentrate on the case of equivariant symmetry. Of considerable importance for the trace formula will be the coadjoint orbit $G \cdot J$ of a momentum vector J. This is the set of points in $\mathcal{G}^*$ that is mapped out when all of the group elements act on J. In the case of rotations, $SO(3) \cdot J$ is the sphere $J = \text{constant}$. It turns out that one can construct a non-degenerate symplectic form for $G \cdot J$, so this space is necessarily even-dimensional. To see this we note that any vector tangent to $G \cdot J$ at J can be written in the form $\mathrm{ad}^*_\xi J$ for some ξ in $\mathcal{G}$, as illustrated in figure 2. The symplectic form is then defined by,

$$\omega(\mathrm{ad}^*_\xi J, \mathrm{ad}^*_\eta J) = J([\xi, \eta]). \tag{4.7}$$

One can easily check that this is well defined and non-degenerate. We let the dimension of $G \cdot J$ be $2l$. For rotations, $l = 1$ when $J \neq 0$ and the symplectic form is proportional to the solid angle 2-form $\sin\theta \, \mathrm{d}\theta \wedge \mathrm{d}\phi$, on the sphere.

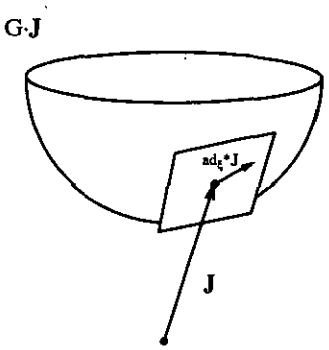

Figure 2. Vectors tangent to the coadjoint orbit $G \cdot J$ at J are all of the form $\mathrm{ad}^*_\xi J$ for some ξ in $\mathcal{G}$. This correspondence allows us to use $\mathcal{G}$-coordinates to parametrize $G \cdot J$ near J.

The following interpretation of the coadjoint orbits might be more familiar from the point of view of physics. The dual space $\mathcal{G}^*$ can be regarded as a phase space in its own right, on which can be defined a Poisson bracket, the so-called Lie-Poisson bracket [4, 12]. In the case of rotational symmetry, $\mathcal{G}^*$ is 3D angular momentum space (coordinates (J_1, J_2, J_3)), and the Poisson bracket is the obvious one, $\{J_a, J_b\} = \varepsilon_{abc} J_c$. The Lie-Poisson bracket is degenerate in that there exist so-called Casimir functions which Poisson-commute with every other function (on $\mathcal{G}^*$)—for example, there is a

single Casimir function J on so(3)*. For any Poisson bracket, if all the Casimir functions are fixed the result is a submanifold on which the Poisson bracket is non-degenerate and in fact can be derived from a symplectic structure. For the Lie-Poisson bracket, the result is just a coadjoint orbit with the symplectic form of (4.7). The codimension $(k-2l)$ of $G\cdot J$ within $\mathcal{G}^*$ is then generically just the number of Casimir functions (there are exceptional cases where the codimension is higher, for example $J=0$).

The dimension of the coadjoint orbit has important consequences for the group structure. Fixing J, we can regard $\mathrm{ad}^*_\xi J$ as a linear map from $\mathcal{G}$ to $\mathcal{G}^*$. The range of $\mathrm{ad}^*_{(\cdot)}J$ is the $2l$-dimensional tangent space to $G\cdot J$ at J and therefore its kernel, $\mathcal{G}_J$ say, is a $(k-2l)$-dimensional subspace of $\mathcal{G}$. The kernel $\mathcal{G}_J$ consists of infinitesimal group elements that leave J fixed and is therefore the tangent space at the identity to the isotropy subgroup G_J of J. G_J is the subgroup of G that leaves J invariant under the coadjoint action. For example, in the case of rotations, G_J is the group of rotations about $\hat{J}$ and $\mathcal{G}_J$ is the space of θ-vectors parallel to $\hat{J}$, each one-dimensional. We will use $\mathcal{G}_J$ to organize coordinates on $\mathcal{G}$ as follows. When considering a point in phase space with a given value of the momentum J, we choose a basis $\{\xi_a\}_{a=1}^k$ for $\mathcal{G}$ in such a way that the first $k-2l$ vectors $\{\xi_a\}_{a=1}^{k-2l}$ form a basis for $\mathcal{G}_J$. The remaining basis vectors $\{\xi_a\}_{a=k-2l+1}^k$ span a $2l$-dimensional subspace, which we will denote by $\mathcal{G}_A$ (A is for active), transverse to $\mathcal{G}_J$. A particular vector ξ can then be decomposed into a component ξ_K in $\mathcal{G}_J$ and a component ξ_A in $\mathcal{G}_A$. We denote by $\theta=(\theta_K,\theta_A)$ the coordinates of a vector ξ relative to this basis. This is a generalization of the $(\theta_\parallel,\theta_\perp)$-decomposition considered in section 3 for rotations.

4.2. *The calculation*

We are now ready to consider the geometry of periodic orbits in phase space. The symmetry of H under G will give rise to $(1+k)$-dimensional families of periodic orbits Γ, parametrized globally by (t, g). We point out that if G is not connected, only the identity component is necessary to parametrize orbits within a given connected family Γ. The different components of G will label a discrete set of different families. As in the previous section, we will concentrate on one connected family at a time, so we will ignore all but the identity component of G. The remaining symmetries are accounted for when we sum discretely over families.

Sufficiently close to any reference orbit γ_0, we can replace the group by the Lie algebra in parametrizing the periodic orbits. This gives rise to local coordinates (t,θ) on Γ, with $\theta=0$ on γ_0. In particular, we choose the coordinates θ to be defined relative to a basis $\{\xi_a\}_{a=1}^k$ that is aligned with the isotropy subgroup of $J_0=J(\gamma_0)$ in the manner described above. Therefore the coordinates on Γ near γ_0 can be decomposed into (t,θ_K,θ_A). These coordinates will enable us to compute the contribution to the integral in (2.3) from an infinitesimal strip around γ_0. To compute the whole integral, we will need to construct such a set of coordinates around every periodic orbit in Γ. The problem with this is that J will vary over Γ so a different basis is needed for $\mathcal{G}$ for each periodic orbit. We need some way to relate the $\mathcal{G}$-bases constructed for different periodic orbits in Γ, and we do this as follows. We first fix a basis $\{\xi_a\}_{a=1}^k$ for the reference orbit γ_0. We then choose the basis corresponding to any other periodic orbit $\gamma_g=g\cdot\gamma_0$ to be $\{g\cdot\xi_a\}_{a=1}^k$. In this way we get a local coordinate system $(t,\theta)=(t,\theta_A,\theta_K)$ about every periodic orbit in Γ. The local coordinates (t,θ) then define a natural measure $\mathrm{d}t\,\mathrm{d}\theta$ on Γ. In terms of the global parametrization (t, g) we can show that this measure coincides with $\mathrm{d}t\,\mathrm{d}\mu_L(g)$, where $\mathrm{d}\mu_L(g)$ is proportional to the

left-invariant measure for G. (For compact groups the left- and right-invariant measures coincide so this distinction need not be made.) We explain this in more detail in appendix B. We will try to interpret the integral in (2.3) in terms of this measure, just as we did for rotational symmetry in section 3.

With this structure in mind, we can proceed to calculate the trace formula. In analogy with the previous section we will define an extended phase space $\tilde{\mathcal{P}} = P \times \mathbb{R} \times G$, with dynamics, $(z', t', g') \to (z = g \cdot \phi_t z', t + t', gg')$ in generalized time (t, g). By methods like those of the previous section, we can then reduce the amplitude $A(\Gamma)$ to the following form,

$$A(\Gamma) = \int_\Gamma \mathrm{d}t \, \mathrm{d}\mu_L(g) \left| \left(\frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta})}{\partial(z'_\perp, \boldsymbol{J}')} \right)_{x_\parallel, x_\parallel, E} \right|^{-1/2}. \tag{4.8}$$

Here we compute $\boldsymbol{J}$ in the basis for $\mathcal{G}^*$ that is dual to the basis $\{\xi_a\}$ of $\mathcal{G}$. In this way the Hamiltonian flow of a particular component $J_a(z)$ generates the action on phase space of the corresponding Lie algebra basis element ξ_a.

As for rotational symmetry, the Jacobian in (4.8) can be interpreted in terms of reduced surface of section mappings. To do this it is necessary to use coordinates for $\mathcal{G}^*$ which take into account the dynamics of $\boldsymbol{J}$. We use any coordinates $(\boldsymbol{B}, \boldsymbol{\beta})$ for $\mathcal{G}^*$, where the $(k-2l)$ coordinates $\boldsymbol{B}$ are constant on each coadjoint orbit $G \cdot \boldsymbol{J}$ (these are the Casimir functions mentioned in section 4.1), providing, in effect, labels for the coadjoint orbits. The remaining $2l$ coordinates $\boldsymbol{\beta}$ then provide coordinate systems on each coadjoint orbit. We will specify a more detailed choice of coordinates later, but for now we let them be relatively arbitrary. These coordinates are a generalization of the coordinates $(J, \hat{\boldsymbol{J}})$ used in the rotational case. Regarded as functions on phase space, we see that the $\boldsymbol{B}$-components are invariant under both H- and G-evolution, whereas G-evolution can carry a given $\boldsymbol{\beta}$ into any other nearby $\boldsymbol{\beta}$. We will choose a surface of section Σ to be a codimension $1+k$ subspace of the $(2n-1-k+2l)$-dimensional level surface $\{z|(H, \boldsymbol{B}) = \text{constant}\}$. To define a surface of section mapping ψ we adjust $1+k$ parameters (t, g) to bring trajectories that start on Σ back to Σ. Note that Σ has dimension $2(n-1-k+l)$, which is even. Σ can therefore be given a symplectic structure by restricting Ω, the full phase space symplectic form, to it. While one might expect that ψ would be symplectic with respect to this structure, it turns out, as mentioned earlier for rotations, that this is not the case. It is the case however, that ψ is symplectic with respect to the following symplectic form on Σ

$$\tilde{\Omega} = \Omega|_\Sigma - \boldsymbol{J}^* \omega \tag{4.9}$$

ω is the symplectic form of (4.7), on the coadjoint orbit $G \cdot \boldsymbol{J}_0$ corresponding to Σ, and $\boldsymbol{J}^*\omega$ is its pull-back using the restricted momentum map $\boldsymbol{J}: \Sigma \to G \cdot \boldsymbol{J}_0$. We show that ψ is symplectic with respect to $\tilde{\Omega}$ in appendix C.

We can interpret the Jacobian of (4.8) in terms of the particular surfaces of section $\Sigma_{\boldsymbol{B}} = \{z|(H, \boldsymbol{B}, x_\parallel) = \text{constant}\}$, with surface of section mappings $\psi_{\boldsymbol{B}}$. As usual, at the periodic orbit family Γ, we use the simpler notation Σ, ψ, etc. We let $z = \psi_{\boldsymbol{B}} z'$ and write,

$$\frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta})}{\partial(z'_\perp, \boldsymbol{J}')} = \frac{\partial(\boldsymbol{\beta}, \boldsymbol{B})}{\partial(\boldsymbol{J})} \left(\frac{\partial \boldsymbol{\theta}_K}{\partial \boldsymbol{B}} \right)_{z_\perp - z'_\perp, \boldsymbol{\theta}_A} \left(\frac{\partial(z_\perp - z'_\perp, \boldsymbol{\theta}_A)}{\partial(z'_\perp, \boldsymbol{\beta}')} \right)_{\boldsymbol{B}} \tag{4.10}$$

by analogy with (3.6). With an appropriate choice for the coordinates $\boldsymbol{\beta}$, the last Jacobian is equal to $\det(M - I)$, where M, as usual, is the Jacobian matrix of ψ at Γ. We construct these coordinates as follows. We have seen that the mapping $\mathrm{ad}^*_{(\cdot)}\boldsymbol{J}$ provides a one-to-one correspondence between the space $\mathcal{G}_A$ and the tangent space of

$G \cdot \boldsymbol{J}$ at $\boldsymbol{J}$. This correspondence allows us to use $\boldsymbol{\theta}_A$ as approximate coordinates on $G \cdot \boldsymbol{J}$ near $\boldsymbol{J}$. Choosing $\boldsymbol{\beta}$ to coincide with the coordinates $\boldsymbol{\theta}_A$ to first order near $\boldsymbol{J}$ we can write,

$$\left(\frac{\partial(\boldsymbol{z}_\perp - \boldsymbol{z}'_\perp, \boldsymbol{\theta}_A)}{\partial(\boldsymbol{z}'_\perp, \boldsymbol{\beta}')}\right)_{\boldsymbol{B}} = \left(\frac{\partial(\boldsymbol{z}_\perp - \boldsymbol{z}'_\perp, \boldsymbol{\beta} - \boldsymbol{\beta}')}{\partial(\boldsymbol{z}'_\perp, \boldsymbol{\beta}')}\right)_{\boldsymbol{B}}$$
$$= \det(M - I) \tag{4.11}$$

where the last equality follows if we use coordinates $(\boldsymbol{z}_\perp, \boldsymbol{\beta})$ on Σ.

The fixed points of the maps $\psi_{\boldsymbol{B}}$ correspond, in phase space, to generalized periodic orbit families $\Gamma_{\boldsymbol{B}}$, consisting of orbits that close after time evolution and a symmetry operation. We expect that the fixed points of $\psi_{\boldsymbol{B}}$ are isolated in each $\Sigma_{\boldsymbol{B}}$, and therefore we get precisely one $(1+k)$-dimensional family $\Gamma_{\boldsymbol{B}}$ for each $\boldsymbol{B}$. These generalized periodic orbits have generalized periods (T, g) whose group part g is in the isotropy subgroup $G_{\boldsymbol{J}}$ at each point on $\Gamma_{\boldsymbol{B}}$. If we consider generalized periodic orbits that are infinitesimally displaced from the periodic orbit family Γ, we can therefore represent the group part of the generalized period by coordinates $\boldsymbol{\Theta} = (0, \boldsymbol{\Theta}_K)$, corresponding to an element of $\mathcal{G}_{\boldsymbol{J}}$. When measured relative to the moving basis $\{g \cdot \xi_a\}$, the coordinates $\boldsymbol{\Theta}_K$ are constant on each $\Gamma_{\boldsymbol{B}}$. This is because, if (T, g_0) is the generalized period of a periodic orbit γ_0 in $\Gamma_{\boldsymbol{B}}$, some other periodic orbit $g \cdot \gamma_0$ has generalized period (T, gg_0g^{-1}). For infinitesimal group periods this conjugation corresponds to the adjoint action of G on $\mathcal{G}$, for which the coordinates $\boldsymbol{\Theta}$ are constant in the moving basis $\{g \cdot \xi_a\}$, which absorbs the action of g on the period. We can therefore write,

$$\left(\frac{\partial \boldsymbol{\theta}_K}{\partial \boldsymbol{B}}\right)_{\boldsymbol{z}_\perp - \boldsymbol{z}'_\perp, \boldsymbol{\theta}_A} = \frac{\partial \boldsymbol{\Theta}_K}{\partial \boldsymbol{B}} \tag{4.12}$$

which is well defined and constant on Γ. It is a direct generalization of (3.11).

The next step is to investigate the term $\partial(\boldsymbol{B}, \boldsymbol{\beta})/\partial(\boldsymbol{J})$ remaining in the integrand of (4.8). This Jacobian for the coordinate change $\boldsymbol{J} \to (\boldsymbol{B}, \boldsymbol{\beta})$ on $\mathcal{G}^*$ is determined by the volume of the $(\boldsymbol{\beta}, \boldsymbol{B})$ coordinate basis (e_β, e_B) relative to the global vector coordinates $\boldsymbol{J}$. For the choice of coordinates $\boldsymbol{\beta}$ outlined above, the $2l$ vectors e_β are given at some point $\boldsymbol{J}_0$ in $\mathcal{G}^*$ by $\mathrm{ad}^*_{\xi_a}\boldsymbol{J}_0$ along $G \cdot \boldsymbol{J}_0$, where $k - 2l + 1 \leq a \leq k$. The remaining $k - 2l$ vectors e_B are unit-$\boldsymbol{B}$ vectors transverse to $G \cdot \boldsymbol{J}_0$ that point to different coadjoint orbits. At another point $g \cdot \boldsymbol{J}_0$, for which one uses a basis $\{g \cdot \xi_a\}$ in $\mathcal{G}$, the vectors e_β are given by $\mathrm{ad}^*_{g\cdot\xi_a} g \cdot \boldsymbol{J}_0 = g \cdot \mathrm{ad}^*_{\xi_a}\boldsymbol{J}_0$ (it can be shown that $g \cdot \mathrm{ad}^*_\xi \boldsymbol{J} = \mathrm{ad}^*_{g\cdot\xi} g \cdot \boldsymbol{J}$ in general). Since g preserves $\boldsymbol{B}$ we can assume without loss of generality that the $\boldsymbol{B}$-coordinate vectors at $g \cdot \boldsymbol{J}_0$ are $g \cdot e_B$. This assumption just amounts to allowing a change of origin in the $\boldsymbol{\beta}$-coordinates as a function of $\boldsymbol{B}$, which will not affect the Jacobian. Therefore the coordinate basis at any point on $G \cdot \boldsymbol{J}_0$ can be expressed in the form $(g \cdot e_\beta, g \cdot e_B)$. Likewise, the coordinate basis vectors $\{\omega^a\}_{a=1}^k$, corresponding to the coordinates $\boldsymbol{J}$, also vary according to $\omega^a \to g \cdot \omega^a$ on Γ. This is an easy consequence of the variation $\xi_a \to g \cdot \xi_a$ of the dual basis $\{\xi_a\}_{a=1}^k$. The net effect is that the Jacobian $\partial(\boldsymbol{B}, \boldsymbol{\beta})/\partial \boldsymbol{J}$ remains unchanged as we consider different points on $G \cdot \boldsymbol{J}$. Let us denote $\partial(\boldsymbol{B}, \boldsymbol{\beta})/\partial \boldsymbol{J}$ by $Q_0(\boldsymbol{B})$. This constant term can now be removed from the integral for $A(\Gamma)$ and all that is left is a normalization of the volume element $\mathrm{d}t\, \mathrm{d}\mu_L(g)$ over Γ.

So far we have assumed that the $\boldsymbol{B}$-coordinates are globally constant on $G \cdot \boldsymbol{J}$. If we single out a particular momentum vector $\boldsymbol{J}_0$, we can use coordinates which, while not rigorously constant on all of $G \cdot \boldsymbol{J}$, are constant in a linearized sense for small variations away from $\boldsymbol{J}_0$ on $G \cdot \boldsymbol{J}$. That is, the Jacobians in 4.10 are unchanged if we

replace $\boldsymbol{B}$ with linear coordinates on $\mathcal{G}^*$ that are constant on the tangent space to $G \cdot \boldsymbol{J}$ at $\boldsymbol{J}$. The basis $\{\xi_a\}_{a=1}^k$ on $\mathcal{G}$ gives us such a set of coordinates in a natural way when the basis is aligned with G_{J_0} in the manner described earlier. This basis defines a set of coordinate functions $\{J_a\}_{a=1}^k$ on $\mathcal{G}^*$. Let us denote the first $k-2l$ of these by $\boldsymbol{J}_K$, and the last $2l$ by $\boldsymbol{J}_A$. It is not difficult to check that $\boldsymbol{J}_K = 0$ along any vector of the form $\mathrm{ad}^*_\xi \boldsymbol{J}_0$ in $\mathcal{G}^*$, that is, that $\boldsymbol{J}_K$ is constant along the tangent space $T_{J_0} G \cdot \boldsymbol{J}$ to $G \cdot \boldsymbol{J}$ at $\boldsymbol{J}_0$. We illustrate this schematically in figure 3. With this choice for $\boldsymbol{B}$, and with the choice of $\boldsymbol{\theta}_A$ for $\boldsymbol{\beta}$ outlined above, we can then write,

$$Q_0 = \frac{\partial(\boldsymbol{B}, \boldsymbol{\beta})}{\partial(\boldsymbol{J})} = \frac{\partial(\boldsymbol{J}_K, \boldsymbol{\theta}_A)}{\partial(\boldsymbol{J}_K, \boldsymbol{J}_A)} = \left(\frac{\partial \boldsymbol{J}_A}{\partial \boldsymbol{\theta}_A}\right)^{-1}_{\boldsymbol{J}_K}. \tag{4.13}$$

Keeping $\boldsymbol{J}_K$ fixed in this last Jacobian amounts to restricting ourselves to the tangent space $T_{J_0} G \cdot \boldsymbol{J}$. We can then interpret $Q_0^{-1} = \partial \boldsymbol{J}_A / \partial \boldsymbol{\theta}_A$ as a Jacobian for the transformation $\mathrm{ad}^*_{(\cdot)} \boldsymbol{J}_0 : \mathcal{G}_A \to T_{J_0} G \cdot \boldsymbol{J}$, in which we use coordinates $\boldsymbol{\theta}_A$ on $\mathcal{G}_A$ and coordinates $\boldsymbol{J}_A$ on $T_{J_0} G \cdot \boldsymbol{J}$. In a similar vein, we can reinterpret the Jacobian of (4.12) as follows,

$$\partial \boldsymbol{\Theta}_K / \partial \boldsymbol{B} = \partial \boldsymbol{\Theta}_K / \partial \boldsymbol{J}_K \tag{4.14}$$

in terms of these local coordinates.

We have shown that the integrand of (4.8) is constant with respect to the volume element $\mathrm{d}t\, \mathrm{d}\mu_L(g)$. Let us denote the remaining integral over Γ by,

$$\int_\Gamma \mathrm{d}t\, \mathrm{d}\mu_L(g) = T_0 V_0 \tag{4.15}$$

where T_0 is the period of a primitive periodic orbit in Γ and V_0 is the integral of $\mathrm{d}\mu_L(g)$ over Γ. In the case of compact groups G we can write, in analogy with (4.14),

$$V_0 = \frac{C_G}{N_I} \tag{4.16}$$

where C_G is the normalization of the measure $\mathrm{d}\mu_L(g) = \mathrm{d}\mu_R(g)$ over the whole group G and N_I is the number of group elements that bring a given periodic orbit in Γ back to itself. If the group is not compact, the measure $\mathrm{d}\mu_L(g)$ is not normalizable on G

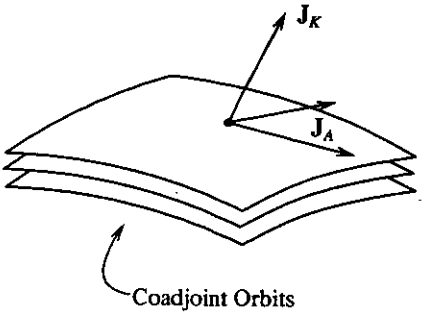

Figure 3. The linear coordinates $\boldsymbol{J}_A$ are locally parallel to the coadjoint orbits near $\boldsymbol{J}$ and are therefore good local coordinates on a particular orbit, providing an alternative to the coordinates $\boldsymbol{\theta}_A$. The linear coordinates $\boldsymbol{J}_K$ point away from $G \cdot \boldsymbol{J}$ and provide a parametrization of nearby coadjoint orbits. $\boldsymbol{J}_K$ can therefore replace the global coordinates $\boldsymbol{B}$ near $\boldsymbol{J}$.

we have to be more careful. If $I(\gamma)$ is the discrete subgroup of G that leaves a periodic orbit γ in Γ invariant, then V_0 is the normalization of $d\mu_L(g)$ over the quotient space $G/I(\gamma)$. Note that $I(\gamma)$ need not be a normal subgroup of G so $G/I(\gamma)$ is not generally a group.

We have derived the following trace formula for systems with general symmetries,

$$g(E) \approx \frac{1}{i\hbar} \frac{1}{(2\pi i\hbar)^{k/2}} \sum_{\Gamma} \frac{T_0 V_0 \exp\left(\frac{i}{\hbar} S(E) - i\sigma\pi/2\right)}{|Q_0|^{1/2} |\partial\Theta_K/\partial J_K|^{1/2} |\det(M-I)|^{1/2}} \tag{4.17}$$

in which, as usual, the various contributing terms are coordinate-free, invariant properties of the periodic orbit families Γ. In the special cases of Abelian and rotational symmetries this trace formula reduces to (1.1) and (3.15) respectively.

5. Conclusion

Equation (4.17), along with the modified versions in the appendices, achieves the goal of finding a generalization of Gutzwiller's trace formula that is valid for systems with arbitrary symmetry. In terms of the density of states, we can restate (4.17) as follows,

$$\rho_{osc}(E) \approx \frac{1}{\pi\hbar} \frac{1}{(2\pi\hbar)^{k/2}} \sum_{\substack{\text{periodic} \\ \text{orbit} \\ \text{families}}} \frac{T_0 V_0 \cos\left(\frac{S}{\hbar} - \frac{\sigma\pi}{2} - \frac{k\pi}{4}\right)}{|Q_0|^{1/2} |\partial\Theta_K/\partial J_K|^{1/2} |\det(M-I)|^{1/2}} \tag{5.1}$$

where $\rho_{osc}(E)$ is the oscillatory part of the density of states. This follows from the trace formulae for $g(E)$ and from $\rho_{osc}(E) = -(1/\pi)\,\mathrm{Im}\, g(E)$. In the special case of Abelian symmetry considered in I, $Q_0 = 1$ and $\partial\Theta_K/\partial J_K = \partial\Theta/\partial J$. For rotational symmetry, $Q_0 = J^{-2}$ and $\partial\Theta_K/\partial J_K = \partial\Theta_\parallel/\partial J$.

Equation (5.1) gives the density of states that corresponds to the complete set of energy levels of the Hamiltonian H. When there is a symmetry present, one can also consider just the energy levels that correspond to a given symmetry class. That is, the spectrum can be broken up into components that correspond to irreducible representations, which we label by j, of the symmetry group and we can consider a reduced density of states $\rho_j(E)$ for each j. It is then reasonable to consider trace formulae for each reduced density of states $\rho_j(E)$. We expect that such a trace formula will determine $\rho_j(E)$ in terms of the classically reduced dynamics. As shown by Robbins [14], this is already known to be true for discrete symmetries. Also, in specific cases of continuous symmetry, such as axial symmetry, simple direct arguments show this to be the case [1, 15, 16]. Such a connection is reasonable because the irreducible representation labels j, can be interpreted semiclassically (in fact, the interpretation can be made exact) as labels for the coadjoint orbits in $\mathcal{G}^*$ [17]. For example, in rotational symmetry, the angular momentum quantum number j corresponds to a classical magnitude of total angular momentum $J = (j + 1/2)\hbar$. The coadjoint orbits in turn label the classically reduced phase spaces [4, 12], so we can establish a one-to-one correspondence between labels j and particular reduced phase spaces, whose periodic orbits would determine $\rho_j(E)$.

The calculations for the reduced densities of states are clearly important and we will discuss them in a future publication. We would like to point out however, that

the full density of states $\rho(E)$ is important in its own right, and that there are instances where a trace formula for $\rho(E)$ rather than for $\rho_j(E)$ is the relevant object to study. For example, it is the density of states for the full spectrum, not the spectrum for a given angular momentum quantum number, that is relevant for the study of nuclear shell structure [5–7]. The results described in section 4 for rotational symmetry are relevant for these calculations. Determining of the whole spectrum at once, as described in this paper, rather than through partial sums for the reduced densities of states, is desirable for these kinds of calculations because only orbits that are periodic in full phase space are required. In contrast, the sums for the reduced densities of states require knowledge of all orbits that are periodic in reduced phase space. The results of this paper provide a means of bypassing all but a small subset of these orbits.

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Appendix A

In this appendix we give a brief outline of the calculation of $A(\Gamma)$ in the case $1+k>n$. The calculations presented here are not meant to be comprehensive. We present only the main ideas; the steps in between can be completed with calculations that are similar to those presented in the main text.

Suppose $1+k>n$. Then, over a given point x in configuration space, we expect that Γ will determine a $(1+k-n)$-dimensional surface in momentum space. Construct momentum space coordinates $(p_\parallel, p_\perp)$ such that the $(1+k-n)$ $p_\parallel$ coordinates are aligned parallel with this surface and the $(2n-1-k)$ coordinates $p_\perp$ are transverse to it. Let $x_\parallel$ and $x_\perp$ be the corresponding conjugate configuration space variables. Note that this decomposition is *not* the same as the $(\parallel, \perp)$-decomposition considered in the main text. In computing the integral in (2.1), we then use the stationary phase approximation to compute the integral over the $p_\perp$ variables, leaving an integral over $(x', p_\parallel)$ whose phase is stationary everywhere. We can interpret this remaining integral as an integral over the periodic orbit family Γ, on which we use coordinates $(x', p_\perp)$. Following the techniques in I, we arrive at the following analogue of (2.3),

$$A(\Gamma) = \int_\Gamma \mathrm{d}x'\, \mathrm{d}p_\parallel \left| \frac{\partial(x_\perp, p_\parallel, x', E)}{\partial(z', t)} \right|^{-1/2}. \tag{A1}$$

The next step is to re-express this integral in terms of the natural measure $\mathrm{d}t\, \mathrm{d}\theta$. A calculation similar to that preceding (3.4) gives,

$$A(\Gamma) = \int_\Gamma \mathrm{d}t\, \mathrm{d}\theta \left| \left(\frac{\partial(x'_\parallel, \theta)}{\partial(x_\parallel, J')} \right)_{x_\perp, x'_\perp, E, p_\parallel} \right|^{-1/2}. \tag{A2}$$

Now construct a reduced surface of section Σ at some point z_0 on Γ by fixing x, $p_\parallel$, E and B. The dimension of this surface of section is less than that of the

corresponding coadjoint orbit $G \cdot J$ when $1+k > n$, and therefore J maps Σ onto some $2(n-1-k+l)$-dimensional subsurface $J(\Sigma)$ of $G \cdot J$. Choose coordinates $\beta = (\gamma, \delta)$ on $G \cdot J$ such that $\gamma = 0$ on $J(\Sigma)$ and δ are good coordinates for $J(\Sigma)$. Let us further suppose that the coordinates (γ, δ) coincide locally with coordinates defined by letting $\mathrm{ad}_{(\cdot)}J$ act on a basis that is aligned with $\mathscr{G}_J$ as described in section 4. That is, we assume that the basis vectors for the active subspace $\mathscr{G}_A$ can be decomposed into a set $\{\xi_\gamma\}$ and a set $\{\xi_\delta\}$, which generate the γ and δ coordinate directions respectively under the action of $\mathrm{ad}^*_{(\cdot)}$. Denote the associated Lie algebra coordinates by $\theta = (\theta_K, \theta_\gamma, \theta_\delta)$.

The integrand of (A2) can be decomposed as follows,

$$\left(\frac{\partial(\boldsymbol{x}'_\parallel, \boldsymbol{\theta})}{\partial(\boldsymbol{x}_\parallel, \boldsymbol{J}')}\right)_{x_\perp, x'_\perp, E, p_\parallel} = Q_0 \left(\frac{\partial(\boldsymbol{x}'_\parallel, \boldsymbol{\theta}_\gamma, \boldsymbol{\theta}_K)}{\partial(\boldsymbol{x}_\parallel, \boldsymbol{\gamma}', \boldsymbol{B})}\right)_{\theta_\delta, x_\perp, x'_\perp, E, p_\parallel} \left(\frac{\partial \boldsymbol{\theta}_\delta}{\partial \boldsymbol{\delta}'}\right)_{x_\parallel, p_\parallel, x_\perp, x'_\perp, E, \boldsymbol{B}, \gamma'}. \tag{A3}$$

Some further analysis allows one to interpret the individual Jacobians in (A3) in the following way,

$$\left(\frac{\partial(\boldsymbol{x}'_\parallel, \boldsymbol{\theta}_\gamma, \boldsymbol{\theta}_K)}{\partial(\boldsymbol{x}_\parallel, \boldsymbol{\gamma}', \boldsymbol{B})}\right)_{\theta_\delta, x_\perp, x'_\perp, E, p_\parallel} = \frac{\partial \Theta_K}{\partial \boldsymbol{B}} \tag{A4}$$

and,

$$\left(\frac{\partial \boldsymbol{\theta}_\delta}{\partial \boldsymbol{\delta}'}\right)_{x_\parallel, p_\parallel, x_\perp, x'_\perp, E, \boldsymbol{B}, \gamma'} = \det(M - I). \tag{A5}$$

In this way one recovers the results obtained in the main text for the case $1+k \leqslant n$.

Appendix B

In this appendix we show that the local coordinates (t, θ) constructed on Γ, as described in section 4, yield a natural measure $\mathrm{d}t\, \mathrm{d}\theta = \mathrm{d}t\, \mathrm{d}\mu_L(g)$ for Γ. We assume a general symmetry, as in section 4. The results can be specialized to the case of rotational symmetry by interpreting the three vectors ξ_a as orthonormal basis vectors for $\mathbb{R}^3$ and $\exp(\theta^a \xi_a)$ as a rotation about direction $\theta^a \xi_a$ by angle $|\theta_a \xi_a|$.

Suppose first that the local coordinates (t, θ) are constructed on Γ with the help of a fixed basis $\{\xi_a\}$ for $\mathscr{G}$. Let $\{Y_a(g)\}$ be the basis obtained for the tangent space of G at each point g by right translation of $\{\xi_a\}$ from the identity. We define a measure $\mathrm{d}\mu_R(g)$ on G, relative to which the volume of the parallelepiped defined by $\{Y_a(g)\}$ is equal to 1 for each g. If we coordinatize G near g according to $g(\theta) = \exp(\theta^a \xi_a) g$, then $\mathrm{d}\mu_R = \mathrm{d}\theta$ at g. This measure is obviously invariant under right translation and can therefore be taken as the right-invariant measure for G. Suppose now that, near a point $g \cdot z_0(t)$ on the periodic orbit $g \cdot \gamma_0$, we define local coordinates (t, θ) for Γ according to $z(t, \theta) = \exp(\theta^a \xi_a) g \cdot z_0(t)$. Then from the preceding discussion we see that $\mathrm{d}t\, \mathrm{d}\theta = \mathrm{d}t\, \mathrm{d}\mu_R(g)$ at $g \cdot \gamma_0$.

In reality however, we do not keep the basis $\{\xi_a\}$ fixed but rather move it around with the adjoint action, so that the components θ^a are defined with respect to the basis $\{\mathrm{Ad}_g \xi_a\}$ at $g \cdot \gamma_0$. It is not difficult to see from the definition of the adjoint action that right-translating the basis $\{\mathrm{Ad}_g \xi_a\}$ to g is the same as left-translating $\{\xi_a\}$ to g and therefore defines a left- rather than a right-invariant measure $\mathrm{d}\mu_L(g)$. (As an aside we note that it is easy to see from this that the left- and right-invariant measures are related through $\mathrm{d}\mu_R(g) = \det \mathrm{Ad}_g\, \mathrm{d}\mu_L(g)$.) It follows that, with $\mathrm{d}\theta$ as constructed in section 4, $\mathrm{d}t\, \mathrm{d}\theta = \mathrm{d}t\, \mathrm{d}\mu_L(g)$ as asserted.

Appendix C

In this appendix we will investigate the symplectic structure of the reduced surface of section mappings ψ. We use the terminology and notation of the general case, described in section 4. While ψ is derived from symplectic mappings ϕ_{tg}, defined by $\phi_{tg}z = g \cdot \phi_t z$, we find that ψ is not necessarily itself symplectic, at least not with respect to the symplectic structure one would most straightforwardly associate with Σ, namely $\Omega|_\Sigma$. This is in contrast to the mappings considered in I, which were symplectic with respect to $\Omega|_\Sigma$. We will find however that there is an alternative symplectic structure on Σ, given by (4.9), with respect to which ψ is symplectic.

The map ψ is symplectic with respect to $\Omega|_\Sigma$ if the following identity holds for any two vectors u and v tangent to Σ at some point z,

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

Here we let $\psi_* u$ denote the linearized propagation of u by the map ψ. The propagation of these vectors by ψ is related to the propagation by the constant (t, g) mapping ϕ_{tg} according to

$$\psi_* w = \phi_{tg*} w + \mathrm{d}t(w) X_H + \mathrm{d}\theta^a(w) X_{J_a}. \tag{C2}$$

An analogous formula is discussed fully in I. We let X_H and X_{J_a} denote the Hamiltonian vector fields for H and J_a respectively, while $\mathrm{d}t(w)$ and $\mathrm{d}\theta^a(w)$ represent the additional (infinitesimal) time evolution and symmetry operation necessary to bring the tip of w back to Σ after propagation by ϕ_{tg}. Inserting (C2) into condition (C1), we get,

$$\Omega(\psi_* u, \psi_* v) = \Omega(u, v) + \{J_a, J_b\}\, \mathrm{d}\theta^a(u)\, \mathrm{d}\theta^b(v) + \mathrm{d}\theta^a(u)\, \mathrm{d}J_a(\phi_{tg*} v) - \mathrm{d}\theta^a(v)\, \mathrm{d}J_a(\phi_{tg*} u). \tag{C3}$$

Note that for the mappings considered in I, for which J is constant on Σ and $\{J_a, J_b\} = 0$, (C3) automatically reduces to (C1) and ψ is symplectic. More generally however J varies along Σ and $\{J_a, J_b\} \neq 0$, so ψ is not obviously symplectic. In the general case we denote the discrepancy between $\Omega(\psi_* u, \psi_* v)$ and $\Omega(u, v)$ by $\alpha(u, v)$. Then $\alpha(u, v)$ can be expressed in a form that is independent of the basis $\{\xi_a\}$ for $\mathcal{G}$ as follows,

$$\alpha(u, v) = \langle \mathrm{d}\boldsymbol{J}(\phi_{tg*} v), \theta(u)\rangle - \langle \mathrm{d}\boldsymbol{J}(\phi_{tg*} u), \theta(v)\rangle + \langle \boldsymbol{J}(\psi z), [\theta(u), \theta(v)]\rangle \tag{C4}$$

where, by an abuse of notation, we let $\theta(w) = \mathrm{d}\theta^a(w)\xi_a$ and make use of the fact that, for equivariant actions, $\{J_a, J_b\}\, \mathrm{d}\theta^a(u)\, \mathrm{d}\theta^b(v) = \boldsymbol{J}([\theta(u), \theta(v)])$ [4].

Note now that it is inherent in the definition of Σ that, when evaluated on Σ, $\boldsymbol{J}$ is restricted to a single coadjoint orbit. The variation of $\boldsymbol{J}$ along Σ can therefore be achieved by applying a group action to $\boldsymbol{J}$. That is, for each z and z' in Σ, there is a $g(z, z')$ such that $\boldsymbol{J}(z) = g(z, z') \cdot \boldsymbol{J}(z')$. The infinitesimal version of this is that the variation of $\boldsymbol{J}$ along some vector u tangent to Σ at a point z is given by,

$$\mathrm{d}\boldsymbol{J}(u) = \mathrm{ad}^*_{\xi(u)} \boldsymbol{J}(z) \tag{C5}$$

for some $\xi(u)$ in $\mathcal{G}$ that can be chosen linear in u. The variation along the propagated vector $\phi_{tg*} u$ is related to this according to,

$$\begin{aligned} \mathrm{d}\boldsymbol{J}(\phi_{tg*} u) &= g \cdot \mathrm{d}\boldsymbol{J}(u) \\ &= g \cdot \mathrm{ad}^*_{\xi(u)} \boldsymbol{J}(z) \\ &= \mathrm{ad}^*_{g \cdot \xi(u)} \boldsymbol{J}(\psi z). \end{aligned} \tag{C6}$$

Substituting this into (C4) and making use of the identity $\langle \mathrm{ad}^*_\eta J, \xi\rangle = \langle J, [\xi, \eta]\rangle$, we can write,

$$\alpha(u, v) = \langle J(\psi z), [\theta(u), g\cdot\xi(v)] + [g\cdot\xi(u), \theta(v)] + [\theta(u), \theta(v)]\rangle. \tag{C7}$$

If $\mathrm{d}J(u)$ is the variation of J along u, the variation along $\psi_* u$ is given by

$$\mathrm{d}J(\psi_* u) = g\cdot \mathrm{d}J(u) + \mathrm{ad}^*_{\theta(u)} J(\psi z) \tag{C8}$$

which, when combined with (C5), yields

$$\mathrm{ad}^*_{\theta(u)+g\cdot\xi(u)-\xi(\psi_* u)} J(\psi z) = 0. \tag{C9}$$

We can use this identity to eliminate $\theta(u)$ and $\theta(v)$ from (C7) giving, after some manipulation,

$$\alpha(u, v) = \langle J(\psi z), [\xi(\psi_* u), \xi(\psi_* v)] - [g\cdot\xi(u), g\cdot\xi(v)]\rangle. \tag{C10}$$

With the identity $[g\cdot\xi, g\cdot\eta] = g\cdot[\xi, \eta]$ [4], we can further reduce this to

$$\begin{aligned}\alpha(u, v) &= \langle J(\psi z), [\xi(\psi_* u), \xi(\psi_* v)]\rangle - \langle g^{-1}\cdot J(\psi z), [\xi(u), \xi(v)]\rangle \\ &= \langle J(\psi z), [\xi(\psi_* u), \xi(\psi_* v)]\rangle - \langle J(z), [\xi(u), \xi(v)]\rangle\end{aligned} \tag{C11}$$

which is clearly related to the symplectic form ω of (4.7), defined on a coadjoint orbit in $\mathcal{G}^*$. Two vectors u and v along Σ define, through (C5), a corresponding pair of vectors along a coadjoint orbit in $\mathcal{G}^*$, to which we can apply the symplectic form ω as follows,

$$J^*\omega(u, v) = \omega(\mathrm{d}J(u), \mathrm{d}J(v)) = \langle J, [\xi(u), \xi(v)]\rangle. \tag{C12}$$

We therefore find from (C11) that

$$\Omega(\psi_* u, \psi_* v) - J^*\omega(\psi_* u, \psi_* v) = \Omega(u, v) - J^*\omega(u, v) \tag{C13}$$

i.e., that ψ is symplectic with respect to the symplectic form $\tilde{\Omega} = \Omega|_\Sigma - J^*\omega$ on Σ, as asserted. There is an important special case where $\tilde{\Omega}$ reduces simply to Ω, and that is when Σ is chosen to lie in a level set of J. In this case $\mathrm{d}J(u) = 0$ and therefore $J^*\omega = 0$. More generally, however, $J^*\omega \neq 0$ and one needs to use the full structure of $\tilde{\Omega}$ in order that ψ be symplectic.

Finally, we note that the reduced surface of section considered here, and the symplectic structure defined by $\tilde{\Omega}$, are closely related to the so-called orbit reduction procedure of Marle [18] and Kazhdan *et al* [19]. In this procedure, one first restricts phase space dynamics to a level surface on which J is constrained to a coadjoint orbit and then identifies points related by a symmetry in G. The resulting quotient space can be made into a symplectic manifold with a symplectic form similar to $\tilde{\Omega}$. The reduced surface of section considered here projects to a regular surface of section in this reduced phase space.

Appendix D

Throughout this paper, we have assumed that the action of the symmetry group G on phase space is locally free. That is, we have assumed that the infinitesimal generators $(\xi_a)_P$ for the group action are linearly independent. We have also assumed that the Hamiltonian vector field X_H is linearly independent of the $(\xi_a)_P$'s. This is not always the case in systems of physical interest. For example, the hydrogen atom has the 6D

symmetry group SO(4), and the six infinitesimal generators for this symmetry cannot be linearly independent on the 5D energy shell [20]. A similar argument applies to the n-dimensional isotropic harmonic oscillator, which has the n^2-dimensional symmetry group U(n) [20].

In this appendix we will discuss how the results presented in the main text are to be modified for these systems. Stated in terms of the global group structure, the systems we want to consider are those for which the isotropy subgroup G_p of a typical point p in P is a continuous group. G_p consists of those elements of G that leave p fixed. The linear dependence of the infinitesimal generators of G can be described by the fact that the infinitesimal generators of G_p vanish at p. We will assume in this appendix that G_p is m-dimensional. We will also assume initially that the Hamiltonian flow is independent of the symmetry. We find then that when the whole group acts on p, a $(k-m)$-dimensional manifold is swept out and that periodic orbit families correspond to $(1+k-m)$-dimensional manifolds in phase space. Periodic orbits in a family Γ are parametrized by the $(k-m)$-dimensional space of left cosets $\tilde{G}=G/G_p$. Notice that G_p is not necessarily a normal subgroup of G, in which case $\tilde{G}$ cannot be made into a group. Notice also that the group G_p varies over Γ according to $G_{g\cdot p}=gG_pg^{-1}$, however these isotropy subgroups are isomorphic to each other, and the differences between them just amount to a relabelling of points.

We denote by $\mathcal{G}_p$ the m-dimensional subalgebra of $\mathcal{G}$ that corresponds to G_p. If G_p preserves p, it certainly preserves the momentum $\boldsymbol{J}$ of p. We find therefore that G_p is a subgroup of G_J, where G_J is the $(k-2l)$-dimensional isotropy subgroup of $\boldsymbol{J}$ under the coadjoint action of G on $\mathcal{G}^*$. We also find then that $\mathcal{G}_p$ is a subalgebra of $\mathcal{G}_J$. We therefore have the following hierarchy of Lie-algebras within $\mathcal{G}$,

$$\mathcal{G}_p \leqslant \mathcal{G}_J \leqslant \mathcal{G}. \tag{D1}$$

We will use this hierarchy of Lie algebras to organize a basis for $\mathcal{G}$ as follows. We construct a basis $\{\xi_a\}_{a=1}^{k}$ for which the first m vectors span $\mathcal{G}_p$, and the first $k-2l$ vectors span $\mathcal{G}_J$. We denote by $\tilde{\mathcal{G}}_J$, the subspace of $\mathcal{G}_J$ spanned by the vectors ξ_a with $m<a\leqslant k-2l$, and we denote by $\tilde{\mathcal{G}}$ the subspace spanned by the vectors with $m<a\leqslant k$. The spaces $\tilde{\mathcal{G}}_J$ and $\tilde{\mathcal{G}}$ are isomorphic with the quotient spaces $\mathcal{G}_J/\mathcal{G}_p$ and $\mathcal{G}/\mathcal{G}_p$, respectively. As before, we let $\mathcal{G}_A$ denote the space spanned by $\{\xi_a | k-2l<a\leqslant k\}$. We decompose the coordinates on $\mathcal{G}$ corresponding to this basis according to, $\boldsymbol{\theta}=(\boldsymbol{\theta}_I, \tilde{\boldsymbol{\theta}}_K, \boldsymbol{\theta}_A)$, where $\boldsymbol{\theta}_I$ are coordinates on $\mathcal{G}_p$, $\tilde{\boldsymbol{\theta}}_K$ are coordinates on $\tilde{\mathcal{G}}_J$, and $\boldsymbol{\theta}_A$ are coordinates on $\mathcal{G}_A$. We further denote $\tilde{\boldsymbol{\theta}}=(\tilde{\boldsymbol{\theta}}_K, \boldsymbol{\theta}_A)$, which are coordinates on $\tilde{\mathcal{G}}$.

The coordinates $\tilde{\boldsymbol{\theta}}$ are to be interpreted as local coordinates on the coset space $\tilde{G}$. As such they give a local parametrization of the periodic orbits in the family Γ near a reference orbit γ_0. Denote the last $k-m$ components of $\boldsymbol{J}$ collectively by $\tilde{\boldsymbol{J}}$. Each of these components generates, as its Hamiltonian vector field, an infinitesimal generator on phase space of one of the basis elements of $\tilde{\mathcal{G}}$, so the $\tilde{\boldsymbol{\theta}}$ coordinates on Γ can be interpreted as evolution parameters for the Hamiltonians $\tilde{\boldsymbol{J}}$. One can now repeat the analysis leading up to (4.8), replacing $\boldsymbol{\theta}$ everywhere by $\tilde{\boldsymbol{\theta}}$, and $\boldsymbol{J}$ by $\tilde{\boldsymbol{J}}$. The result is

$$A(\Gamma)=\int_{\Gamma} \mathrm{d}t\, \mathrm{d}\tilde{\boldsymbol{\theta}} \left| \left(\frac{\partial(\boldsymbol{z}_\perp - \boldsymbol{z}'_\perp, \tilde{\boldsymbol{\theta}})}{\partial(\boldsymbol{z}'_\perp, \tilde{\boldsymbol{J}}')} \right)_{x'_\parallel, x_\parallel, E} \right|^{-1/2}. \tag{D2}$$

The volume element $\mathrm{d}\tilde{\boldsymbol{\theta}}$ can be interpreted as coming from a projection of the left invariant measure $\mathrm{d}\mu_L(g)$ of G onto the coset space $\tilde{G}$.

The next step is to interpret this modified version of (4.8) in terms of reduced surface of section mappings. The first thing to notice is that the components of $\boldsymbol{J}$ are

not all functionally independent. In fact, the gradients of the first m components of $\boldsymbol{J}$ vanish at p because their Hamiltonian vector fields, which are infinitesimal generators for $\mathcal{G}_p$, vanish at p. (Notice that G_p, and therefore the coordinate system on $\mathcal{G}^*$ from which these components are taken, will vary with p.) Therefore $\boldsymbol{J}$ represents just $k-m$ independent conditions on phase space, and this implies that $\boldsymbol{J}$ maps all of phase space onto a $(k-m)$-dimensional submanifold $\boldsymbol{J}(P)$ of the k-dimensional space $\mathcal{G}^*$, at least locally. The tangent space to $\boldsymbol{J}(P)$ at $\boldsymbol{J}(p)$ is specified by fixing the first m components of $\boldsymbol{J}$. G leaves $\boldsymbol{J}(P)$ invariant, so $\boldsymbol{J}(P)$ forms a $(k-m-2l)$-parameter family of coadjoint orbits. In constructing the coordinates $(\boldsymbol{B}, \boldsymbol{\beta})$ described in section 4, let us choose $\boldsymbol{B}$ to consist of $k-m-2l$ coordinates $\boldsymbol{C}$ and m coordinates $\boldsymbol{D}$, constructed in such a way that $\boldsymbol{J}(P)$ is specified by the condition $\boldsymbol{D}=0$. In this way, the coordinates $\boldsymbol{C}$ label the coadjoint orbits within $\boldsymbol{J}(P)$ and the $k-m$ coordinates $(\boldsymbol{C}, \boldsymbol{\beta})$ are functionally independent on P. We will take the reduced surface of section to lie in a $(2n-1-k+m+2l)$-dimensional invariant level surface of $(H, \boldsymbol{C})$. We take for the surface of section Σ, any codimension $1+k-m$ subspace of this level surface. Time evolution and symmetry operations then give $1+k-m$ independent parameters with which to make trajectories intersect Σ. This leads to a surface of section map ψ of $n-1-k+m+l$ degrees of freedom.

As mentioned previously, the construction of the $\tilde{\boldsymbol{J}}$ coordinates depends on the subgroup G_p, which in turn depends on p. Therefore the $\tilde{\boldsymbol{J}}$ functions (as well as the $\tilde{\boldsymbol{\theta}}$ coordinates) occurring in (D2) have to be redefined at each point on Γ as the integral is summed. For this reason, it is not possible to use the global coordinates $(\boldsymbol{B}, \boldsymbol{\beta})$ in the same way that they are used in section 4, as, for example, in (4.10). Instead, we must switch straight away to local coordinates $\tilde{\boldsymbol{J}} = (\tilde{\boldsymbol{J}}_{\mathrm{K}}, \boldsymbol{J}_{\mathrm{A}})$, analogous to the coordinates $\boldsymbol{J} = (\boldsymbol{J}_{\mathrm{K}}, \boldsymbol{J}_{\mathrm{A}})$ appearing in (4.13) and (4.14). The $\boldsymbol{J}_{\mathrm{A}}$ components are defined as in section 4, corresponding to the last $2l$ basis vectors $\{\xi_a | k-2l < a \leqslant k\}$ and conjugate to the $\boldsymbol{\theta}_{\mathrm{A}}$ coordinates. The components $\tilde{\boldsymbol{J}}_{\mathrm{K}}$ are the last $k-m-2l$ components of $\boldsymbol{J}_{\mathrm{K}}$, corresponding to the basis vectors $\{\xi_a | m < a \leqslant k-2l\}$ and conjugate to the coordinates $\tilde{\boldsymbol{\theta}}_{\mathrm{K}}$. The coordinates $\tilde{\boldsymbol{J}}_{\mathrm{K}}$ are a local replacement for the global coordinates $\boldsymbol{C}$. One can now repeat the rest of the calculations in section 4, with $\tilde{\boldsymbol{J}} = (\tilde{\boldsymbol{J}}_{\mathrm{K}}, \boldsymbol{J}_{\mathrm{A}})$ replacing $\boldsymbol{J} = (\boldsymbol{J}_{\mathrm{K}}, \boldsymbol{J}_{\mathrm{A}})$ and $\tilde{\boldsymbol{\theta}} = (\tilde{\boldsymbol{\theta}}_{\mathrm{K}}, \boldsymbol{\theta}_{\mathrm{A}})$ replacing $\boldsymbol{\theta} = (\boldsymbol{\theta}_{\mathrm{K}}, \boldsymbol{\theta}_{\mathrm{A}})$. The result is the following analogue of (4.17),

$$g(E) \approx \frac{1}{\mathrm{i}\hbar} \frac{1}{(2\pi\mathrm{i}\hbar)^{(k-m)/2}} \sum_{\Gamma} \frac{T_0 \tilde{V}_0 \exp\left(\frac{\mathrm{i}}{\hbar} S(E) - \mathrm{i}\sigma\pi/2\right)}{|Q_0|^{1/2} |\partial \tilde{\boldsymbol{\Theta}}_{\mathrm{K}} / \partial \tilde{\boldsymbol{J}}_{\mathrm{K}}|^{1/2} |\det(M-I)|^{1/2}} \tag{D3}$$

where $T_0 \tilde{V}_0$ is the normalization of $\mathrm{d}t\, \mathrm{d}\tilde{\boldsymbol{\theta}}$ over Γ and Q_0 is still given by (4.13), corresponding to the change of coordinates $\boldsymbol{\theta}_{\mathrm{A}} \to \boldsymbol{J}_{\mathrm{A}}$ on a coadjoint orbit. The group part of the generalized period of a generalized periodic orbit is unique only up to a left coset of G_p, and these are parametrized sufficiently close to the identity by coordinates $\tilde{\boldsymbol{\Theta}}_{\mathrm{K}}$. Finally, we note that for many systems in which the symmetry acts degenerately on phase space, the condition $k-m > n$ holds and a generalization of the calculation of appendix A is more appropriate. The final results are the same however, so we will not discuss this situation further.

In deriving (D3) we assumed that the Hamiltonian flow vector X_H was linearly independent of the infinitesimal generators for the action of G on P. Once again, this condition is not always satisfied for physical systems, and in fact the examples of the hydrogen atom and the isotropic harmonic oscillator mentioned at the beginning of this appendix provide exceptions to this condition. It is therefore important to further

modify (D3) to take these exceptions into account. When X_H can be expressed as a linear combination of infinitesimal generators for G, it means that the net effect of a time evolution on an individual point is the same as the action of some element of G on that point. Therefore, when we let time evolution and group symmetries act on a point, the result is a $(k-m)$-dimensional rather than a $(1+k-m)$-dimensional subspace of P. In particular, a periodic orbit manifold Γ is $(k-m)$-dimensional and the time coordinate t is not independent of the $\tilde{\boldsymbol{\theta}}$ coordinates on Γ described above.

A convenient way to deal with this situation is to treat time evolution and the group symmetry simultaneously in a group $\hat{G}=\mathbb{R}\times G$. An element (t, g) in $\hat{G}$ acts on a point p in P according to $p\to\phi_t g\cdot p$. We will assume that the isotropy subgroup $\hat{G}_p$ of p in $\hat{G}$ is $(m+1)$-dimensional and that $G_p=\hat{G}_p\cap G$ is m-dimensional. We can write the Lie algebra for $\hat{G}$ in the form $\hat{\mathcal{G}}=\mathbb{R}+\mathcal{G}$, and likewise the dual space to the Lie algebra is of the form $\hat{\mathcal{G}}^*=\mathbb{R}+\mathcal{G}^*$.

Corresponding to the action of the whole group $\hat{G}$ on P, there is a momentum map $\boldsymbol{I}$ taking P into covectors in $\hat{\mathcal{G}}^*$. The momentum takes the form $\boldsymbol{I}=(H, \boldsymbol{J})$. Because $\hat{G}_p$ is $(m+1)$-dimensional, $\boldsymbol{I}$ takes phase space into a subspace $\boldsymbol{I}(P)$ of $\hat{\mathcal{G}}^*$ that is of dimension $1+k-(m+1)=k-m$. This follows from the same sort of reasoning as before. The Hamiltonian vector fields generated by the $m+1$ components of $\boldsymbol{I}$ that correspond to the $(m+1)$-dimensional space $\hat{\mathcal{G}}_p$ vanish at p, and therefore the gradients of those components vanish there also. This means that, in a linearized sense, there are only $1+k-(1+m)$ independent components of $\boldsymbol{I}$ at p, and therefore that the tangent space to P at p is mapped into a $(k-m)$-dimensional plane in $\hat{\mathcal{G}}^*$. This implies that, locally, $\boldsymbol{I}(P)$ is a $(k-m)$-dimensional surface in $\mathcal{G}^*$. There are interesting consequences of this for the values of $\boldsymbol{J}$ that can be taken on at a given energy. The intersection of $\boldsymbol{I}(P)$ with the plane $H=E$ in $\hat{\mathcal{G}}^*$ will be $(k-m-1)$-dimensional, and therefore $\boldsymbol{J}$ will map an energy level surface in P into a $(k-m-1)$-dimensional submanifold of $\mathcal{G}^*$. On the other hand, $\boldsymbol{J}$ maps the whole space P into a $(k-m)$-dimensional surface. This is in contrast to the case considered earlier in which the Hamiltonian flow of H is independent of the symmetry, where we found that not only P, but also each energy shell, is mapped onto a $(k-m)$-dimensional surface.

We will employ a basis for $\hat{\mathcal{G}}$ that combines simultaneous displacements in time and along the group G. We choose the first $(m+1)$ vectors to be a basis for $\hat{\mathcal{G}}_p$ and we denote coordinates relative to this basis by $\bar{\boldsymbol{\theta}}_I$. We choose the next $k-2l-m$ vectors in such a way that, along with the first $m+1$ vectors, they span the Lie algebra $\hat{\mathcal{G}}_I$ of the isotropy subgroup of $\boldsymbol{I}$ under the coadjoint action of $\hat{G}$ on $\hat{\mathcal{G}}^*$. It is straightforward to see that $\hat{\mathcal{G}}_I$ is of the form $\hat{\mathcal{G}}_I=\mathbb{R}+\mathcal{G}_J$. In particular we can choose the time direction as one of the vectors and we can choose the remaining $k-2l-m-1$ vectors to lie in $\mathcal{G}$. We denote the $k-2l-m$ coordinates corresponding to these basis vectors by $(t, \bar{\boldsymbol{\theta}}_K)$. Finally, we choose the remaining $2l$ vectors of the $\hat{\mathcal{G}}$-basis to lie in $\mathcal{G}$ and denote the corresponding coordinates by $\boldsymbol{\theta}_A$. We denote the subspaces of $\mathcal{G}$ corresponding to the $\bar{\boldsymbol{\theta}}_K$ and $\boldsymbol{\theta}_A$ coordinates by $\bar{\mathcal{G}}_K$ and $\mathcal{G}_A$ respectively. We denote the corresponding components of $\boldsymbol{J}$ by $\bar{\boldsymbol{J}}=(\bar{\boldsymbol{J}}_K, \boldsymbol{J}_A)$.

The coordinates $(t, \bar{\boldsymbol{\theta}})=(t, \bar{\boldsymbol{\theta}}_K, \boldsymbol{\theta}_A)$ provide a local coordinate system on a periodic orbit manifold Γ, and correspond to evolution parameters for the Hamiltonians $(H, \bar{\boldsymbol{J}})=(H, \bar{\boldsymbol{J}}_K, \boldsymbol{J}_A)$. We can now repeat the calculations described earlier for the case that X_H is independent of the symmetries. The only difference is that $(t, \tilde{\boldsymbol{\theta}})=(t, \tilde{\boldsymbol{\theta}}_K, \boldsymbol{\theta}_A)$ and $(H, \tilde{\boldsymbol{J}})=(H, \tilde{\boldsymbol{J}}_K, \boldsymbol{J}_A)$ should be replaced by $(t, \bar{\boldsymbol{\theta}})=(t, \bar{\boldsymbol{\theta}}_K, \boldsymbol{\theta}_A)$ and $(H, \bar{\boldsymbol{J}})=(H, \bar{\boldsymbol{J}}_K, \boldsymbol{J}_A)$ respectively. For example one arrives at the intermediate result (D2), except with the tildes replaced by overlines. Likewise, the final result is the same as (D3) with overlines

replacing tildes. However, to interpret this final result a brief discussion of reduced surfaces of section is necessary.

Recall that J maps a given energy shell $H=E$ into a $(k-m-1)$-dimensional surface in $\mathcal{G}^*$. Let us construct coordinates $\boldsymbol{B}=(\boldsymbol{C},\boldsymbol{D})$ as before, except that this time setting the $m+1$ coordinates $\boldsymbol{D}=0$ specifies $\boldsymbol{J}(\{H=E\})$ rather than $\boldsymbol{J}(P)$. The remaining $k-2l-m-1$ coordinates $\boldsymbol{C}$ then label the coadjoint orbits within $\boldsymbol{J}(\{H=E\})$. A surface of section Σ will be a codimension $k-m$ subspace of a $(2n-k+m+2l)$-dimensional level surface of $(H,\boldsymbol{C})$. Trajectories are brought back to Σ by adjusting the $k-m$ independent parameters $(t,\bar{\boldsymbol{\theta}})$. This defines a surface of section map ψ of $n-k+l+m$ degrees of freedom. In computing the trace formula in terms of these surfaces of section, we can replace the $\boldsymbol{C}$ coordinates locally by $\bar{\boldsymbol{J}}_{\mathrm{K}}$. In particular, generalized periodic orbit families of a given energy can be parametrized locally by $\bar{\boldsymbol{J}}_{\mathrm{K}}$, which leads to a term $\partial\bar{\boldsymbol{\Theta}}_{\mathrm{K}}/\partial\bar{\boldsymbol{J}}_{\mathrm{K}}$ in the trace formula. Also, the $2l$ components of $\boldsymbol{J}_{\mathrm{A}}$ still provide a convenient local parametrization of points on an individual coadjoint orbit, leading to a Jacobian $Q_0=\partial\boldsymbol{\theta}_{\mathrm{A}}/\partial\boldsymbol{J}_{\mathrm{A}}$ relating these coordinates to the coordinates $\boldsymbol{\theta}_{\mathrm{A}}$ defined through $\mathrm{ad}^*_{(\cdot)}\boldsymbol{J}$.

The resulting trace formula has exactly the same form as (D3), except that tildes are replaced by overlines. Also, of course, the prefactor $(2\pi i\hbar)^{-(k-m)/2}$ is replaced by $(2\pi i\hbar)^{-(k-m-1)/2}$. In light of the preceding discussion, the individual terms can now be interpreted easily.

Appendix E

An arbitrary group action on phase space will not necessarily satisfy the equivariance conditions of (3.1) and (4.6), or the condition $\{J_a,J_b\}=0$ for Abelian symmetries. In this appendix we outline how the calculations presented in the main text of this paper must be modified for this more general case.

It can be shown [4] that any action of a group on phase space is of the following form,

$$\boldsymbol{J}(g\cdot z)=\mathrm{Ad}^*_{g^{-1}}\boldsymbol{J}(z)+\sigma(g) \tag{E1}$$

where $\sigma(g)$, a vector in $\mathcal{G}^*$, is independent of z and satisfies the so-called cocycle identity,

$$\sigma(gh)=\sigma(g)+\mathrm{Ad}^*_{g^{-1}}\sigma(h). \tag{E2}$$

The right-hand side of (E1) defines an action of G on $\mathcal{G}^*$, which we will refer to as the dynamical action and which we denote by $g\cdot\boldsymbol{J}$. Note that this notation is different from that of section 4, where $g\cdot\boldsymbol{J}$ stands for the coadjoint action. We define an infinitesimal version of $\sigma(g)$ according to,

$$\sigma_\xi=\frac{\mathrm{d}}{\mathrm{d}t}\sigma(\exp t\xi)\bigg|_{t=0} \tag{E3}$$

which is linear in ξ.

Like a coadjoint orbit, the orbit $G\cdot\boldsymbol{J}$ of a momentum $\boldsymbol{J}$ under the dynamical action is a symplectic manifold. To see this we note that any vector tangent to $G\cdot\boldsymbol{J}$ at $\boldsymbol{J}$ is of the form,

$$\Delta(\xi)=\mathrm{ad}^*_\xi\boldsymbol{J}+\sigma_\xi \tag{E4}$$

for some ξ in $\mathcal{G}$. We define the symplectic form $\tilde{\omega}$ on $G \cdot J$ according to,

$$\tilde{\omega}(\Delta(\xi), \Delta(\eta)) = \langle J, [\xi, \eta] \rangle. \tag{E5}$$

This is obviously antisymmetric and is easily seen to be well defined and non-degenerate. This symplectic structure forces $G \cdot J$ to be even-dimensional and as before we denote this dimension by $2l$. For fixed J, $\xi \to \Delta(\xi)$ provides a linear mapping from $\mathcal{G}$ onto the tangent space of $G \cdot J$ at J. We denote the $(k-2l)$-dimensional kernel of this mapping by $\mathcal{G}_J$ and let $\mathcal{G}_A$ be a $2l$-*dimensional space transverse to* $\mathcal{G}_J$. Choosing a basis for $\mathcal{G}$ that is aligned with these spaces we can decompose the coordinates of a vector in $\mathcal{G}$ into $\theta = (\theta_K, \theta_A)$, analogous to the construction of section 4.

One can now repeat the analysis of section 4 with this structure in mind, resulting in a trace formula that looks exactly like (4.18) or (5.1). The only difference is that the symbols are interpreted slightly differently, in line with the preceding discussion. In particular one chooses coordinates (B, β) that are constructed around dynamical orbits rather than coadjoint orbits. The Jacobian Q_0 is computed for coordinates β that coincide locally with coordinates θ_A on the tangent space of $G \cdot J$ that are defined by the map Δ of (E4). (Δ carries $\mathcal{G}_A$ isomorphically into the tangent space of $G \cdot J$.) The reduced surfaces of section correspond to a single dynamical orbit and are symplectic with respect to $\Omega|_\Sigma - J^*\tilde{\omega}$. Finally, Θ_K is the group part of the generalized period, defined relative to the basis considered in this appendix.

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