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1993 J. Phys. A: Math. Gen. 26 95

(http://iopscience.iop.org/0305-4470/26/1/013)

J. Phys. A: Math. Gen. 26 (1993) 95–118. Printed in the UK

Semiclassical mechanics of symmetry reduction

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Received 15 June 1992

Abstract. We discuss semiclassical approximations that are adapted to given symmetry classes in quantum mechanics. Arbitrary Abelian symmetries and also rotational symmetry are treated. Semiclassical approximations are derived for the projected propagator and energy dependent Green's function associated with a given irreducible representation of the symmetry group. From these we derive trace formulae, analogous to the usual trace formula, that determine the energy levels in a given symmetry class in terms of classical orbits.

1. Introduction

There has been much interest in recent years in the quantum mechanics of systems whose classical mechanics displays chaos [1, 2]. Much of the interest has been on systems where the classical system, typically with two-degrees of freedom, displays global chaos in phase space. The reason is that systems of this kind are relatively easy to analyse, both numerically and theoretically, while retaining most of the essential features that are of interest in the study of the quantum–classical correspondence.

In this paper, we consider the extension of the semiclassical formalism to an important class of systems not previously amenable to such treatment, except by ad hoc methods—these are systems with continuous symmetry. We consider two types of symmetry in particular—Abelian and rotational—of which there are many examples that occur in practice. These examples range from rotationally symmetric nuclei, atoms, molecules etc., to the axially symmetric electronic motion of diatomic molecules or of free atoms in a magnetic field.

We develop semiclassical approximations appropriate to the restriction of the Schrödinger equation to a subspace associated with a given irreducible representation j of the symmetry group. In sections 3 and 4 we derive approximations for the restricted propagator and Green's function from which the wavefunctions and energy levels in the symmetry class j can in principle be derived [3–6].

While we do not discuss wavefunctions in detail, we do give a detailed discussion of the uses of semiclassical approximations in determining symmetry-reduced spectra. We show how the reduced Green's functions can be used to derive Gutzwiller-like trace formulae, in which each partial density of states $\rho_j(E)$, corresponding to the levels within a given symmetry class j, is determined by a sum over classical orbits. The orbits that determine a reduced spectrum are not periodic in phase space, but they are periodic in a symmetry-reduced phase space, obtained when the appropriate

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0305-4470/93/010095+24$07.50

first integrals have been eliminated. This trace formula complements previous results for the complete density of states of a system with symmetry [7].

We give two interpretations of the sum. The first, presented in section 5, describes the trace formula in terms of the dynamics of full phase space—this is the one that is most directly suggested by the derivation. In this interpretation, a component of the spectrum is determined by a sum over whole families of orbits which close in phase space after some time evolution and also some symmetry operation. This interpretation is strongly connected with the results of [7].

The second interpretation is in terms of the dynamics of reduced phase space, and while it is simpler in form than the full phase space picture, there are ambiguities in the definition of some of the classical quantities occurring in it, such as action integrals (at least when one tries to interpret them solely in terms of reduced dynamics). Nonetheless this version is of interest because it takes the form of a regular Gutzwiller sum applied to the isolated orbits of a reduced phase space, and so it is more directly connected to previous theory. We present this interpretation in section 6.

It should be pointed out that there exist results in the mathematical literature relating trace formulae in the presence of symmetry to the process of classical reduction. In particular, Guillemin and Uribe [8] discuss a trace formula in which the classical input comes from periodic orbits of the symmetry reduced dynamics. Their results are similar to the interpretation of section 6, though in a more abstract setting.

Let us give an outline of the paper. In section 2 we define notation and collect together some of the various facts from group theory that we will use. In section 3 we present a detailed derivation of semiclassical approximations for the reduced Green's functions in the case of arbitrary compact Abelian symmetry. In section 4 we outline how the calculations may be modified for the case of rotational symmetry. In section 5 we show how the reduced energy-dependent Green's function may be used to derive the trace formula for the reduced spectrum. In this section the trace formula is interpreted in terms of dynamics on full phase space and in section 6 we show that the trace formula can also be interpreted in terms of symmetry-reduced phase space. In section 7 we show that the partial densities can be summed to find a trace formula for the full density of states in terms of periodic orbits of full phase space.

2. Some preliminaries

Before getting into the detailed calculations, we begin in this section with a brief overview of the symmetry-related quantities that we are interested in calculating. For additional discussion and motivation we refer the reader to any of the standard group theory references (e.g. [9, 10] and also to the work of Robbins [11] on the case of discrete symmetry, where similar objectives were considered. While we will specialize the calculation in the following sections to the special cases of Abelian and rotational symmetry, it is convenient, for the moment, to keep the discussion general and allow for arbitrary continuous symmetry.

Assuming a compact symmetry group, the irreducible representations can be labelled by a discrete index j, and Hilbert space $\mathcal{H}$ can be correspondingly decomposed into invariant subspaces $\mathcal{H}_j$. Orthogonal projection onto $\mathcal{H}_j$ is achieved by the following operator

$$F_j = d_j \int_G \mathrm{d}\mu(g)\, \chi_j^*(g)\, D(g) \tag{2.1}$$

where $D(g)$ is the unitary operator associated with a symmetry g, χ_j is the character for the jth irreducible representation and $d\mu(g)$ is the invariant or Haar measure on the group, which we assume to be normalized.

Given an operator X that commutes with the symmetry, we form the reduced operator $X_j = F_j X$ acting on $\mathcal{H}_j$. Of particular interest to us are the evolution operator $U(t) = \exp(-iHt/\hbar)$ and the Green's operator $G(E) = 1/E - H$. We define $U_j(t) = F_j U(t)$ and $G_j(E) = F_j G(E)$, for which the x-space matrix elments are

$$K_j(x, x', t) = \langle x|U_j(t)|x'\rangle = \sum_n \exp\left(-\frac{iE_{n,j}t}{\hbar}\right)\psi_{n,j}(x)\psi_{n,j}(x')^* \tag{2.2}$$

and

$$G_j(x, x', E) = \langle x|G_j(E)|x'\rangle = \sum_n \frac{\psi_{n,j}(x)\psi_{n,j}(x')^*}{E - E_{n,j}} \tag{2.3}$$

where $\psi_{n,j}(x)$ and $E_{n,j}$ are, respectively, the wavefunctions and energy levels in the subspace $\mathcal{H}_j$.

3. Green's function for Abelian symmetry

In order to proceed with the calculations outlined in the previous section, it is necessary to understand the group structure of the symmetry in question. For example, in (2.1) it is necessary to know the invariant measure $d\mu(g)$ and, less trivially, the characters $\chi_j(g)$. We will concentrate in this paper on two types of symmetry for which these quantities are trivial or well known—these are Abelian symmetry and rotational symmetry. We expect that the generalization to other symmetries should be straightforward and should not include any novel features, so that the calculations presented here include all the essential structure of the general case, differing in detail only.

We begin in this section with the simplest case of Abelian symmetry, for which we give a detailed derivation of the semiclassical approximations to the Green's function of (2.3). In section 3.1 we first detail some of the exact quantum mechanics and in section 3.2 we go on to consider semiclassical approximations. We leave the rotational case for section 4, where we outline the analogous calculations for that case, which follow the same pattern.

3.1. Some exact quantum mechanics

We begin by summarizing the group structure. We assume that G is compact, connected and k-dimensional, as well as Abelian. (The assumption of connectedness is not important—in the case of non-connected groups we can initially consider the identity component and leave the remaining discrete symmetry for later.) Under these conditions, it is possible to show that G is isomorphic with the torus group T^k, both topologically and group-theoretically.

We can therefore use 2π-periodic coordinates $\theta = (\theta_1, \ldots, \theta_k)$ on G, in terms of which the group multiplication law is given by

$$g(\theta) \cdot g(\theta') = g(\theta + \theta') \tag{3.1}$$

where $\theta + \theta'$ is computed modulo 2π in each component. The irreducible representations are labelled by k-vectors of integers $m = (m_1, \ldots, m_k)$, and the corresponding characters are given by [9]

$$\chi_m(\theta) = \exp(-\mathrm{i}m \cdot \theta) \tag{3.2}$$

(we replace the symbol j by m).

For (2.1) we note that $d_j = 1$ and $\mathrm{d}\mu(g) = (2\pi)^{-k}\mathrm{d}\theta$. We can assume that the symmetry operators $D(\theta)$ are generated by a collection of Hermitian operators $J = (J_1, \ldots, J_k)$ as follows

$$D(\theta) = \exp(-\frac{\mathrm{i}}{\hbar}J \cdot \theta). \tag{3.3}$$

That each $D(\theta)$ must be of this form follows easily by defining $J_a = \mathrm{i}\hbar\partial/\partial\theta_a D(\theta)$ and using the fact that $D(\theta + \theta') = D(\theta)D(\theta')$. In the limit of classical mechanics, the collection of operators J goes over to the collection of first integrals associated with the action of the symmetry group G on phase space by canonical transformations. It is easy to see that the operators J commute with H just as their classical counterparts Poisson commute with the classical Hamiltonian.

We will compute directly the reduced Green's operator $G_m(E)$ from a one-sided Fourier transform of $U_m(t)$ as follows

$$\begin{aligned} G_m(E) &= \frac{1}{\mathrm{i}\hbar}\int_0^\infty \mathrm{d}t\, \exp\left((\mathrm{i}/\hbar)Et\right) U_m(t) \\ &= \frac{1}{\mathrm{i}\hbar}\frac{1}{(2\pi)^k}\int_0^\infty \mathrm{d}t \int_{T^k} \mathrm{d}\theta\, \exp\left((\mathrm{i}/\hbar)Et + \mathrm{i}m \cdot \theta\right) V(t,\theta) \end{aligned} \tag{3.4}$$

where we give E a small positive imaginary part in order to make the time integral converge and define $V(t,\theta) \equiv \exp[-(\mathrm{i}/\hbar)(Ht + J \cdot \theta)]$.

3.2. *Semiclassical approximations*

We now consider semiclassical approximations for the reduced operators. We begin by constructing an approximation for the (t,θ)-evolution operator $V(t,\theta)$, which we will write down by analogy with the usual Van Vleck formula for the propagator. From this approximation it will be possible to compute the reduced Green's function and energy-dependent Green's function by performing Fourier transforms in various combinations of the variables (t,θ), as in (3.4).

Now, we can immediately apply the Van Vleck approximation to $V(t,\theta)$ if we realize that this operator can be interpreted as corresponding the net effect of evolution under Hamiltonian H for time t and the evolutions obtained by using each J_a as a Hamiltonian for time θ_a. The order in which we perform these Hamiltonian evolutions is irrelevant because any two of the operators (H, J) commute. If we denote by $K(x, x', t, \theta)$ the matrix element $\langle x|V(t,\theta)|x'\rangle$ of the (t,θ)-evolution operator, the Van Vleck approximation can be written in the follow way

$$K(x,x',t,\theta) = \frac{1}{(2\pi\mathrm{i}\hbar)^{n/2}}\sum \left|\frac{\partial^2 W}{\partial x \partial x'}\right|^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar}W(x,x',t,\theta) - \mathrm{i}\frac{\mu\pi}{2}\right). \tag{3.5}$$

Here, the sum is taken over classical trajectories that start at position x' and end at position x in configuration space after flowing under the Hamiltonian dynamics of H for time t and each conserved quantity J_a for time θ_a. Also, n is the number of degrees of freedom and μ is the Maslov index. $W(x,x',t,\theta)$ is a generalization of Hamilton's principal function that is appropriate for the (t,θ) path

$$W(x,x',t,\theta) = \int_{t-\text{path}} p\cdot dx - H dt + \int_{\theta-\text{path}} p\cdot dx - J\cdot d\theta. \quad (3.6)$$

This action is independent of the order in which the individual parts of the t- and θ-evolutions are performed, just as the quantum mechanical operator $V(t,\theta)$ is.

We will find it very useful to interpret $W(x,x',t,\theta)$ as a wavefunction on an extended Hilbert space $\mathcal{H}_{\text{ext}} = L^2(\mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^k)$, consisting of functions of the $(n+1+k)$ variables (x,t,θ). We regard x' as a parameter. (Technically, of course, $K(x,x',t,\theta)$ is not an element of $\mathcal{H}_{\text{ext}}$ because it is not square-integrable in the t coordinate, but this detail is not important.) In the classical limit, $\mathcal{H}_{\text{ext}}$ is replaced by an extended phase space $P_{\text{ext}} = P\times\mathbb{R}^2\times\mathbb{R}^{2k}$, with canonical coordinates (x,p,t,h,θ,j) and a symplectic form

$$\Omega_{\text{ext}} = dx\wedge dp + dt\wedge dh + d\theta\wedge dj. \quad (3.7)$$

We generate t-dynamics on P_{ext} with the extended Hamiltonian $H_{\text{ext}} = H(x,p) + h$ and θ-dynamics with the collection of Hamiltonians $J_{\text{ext}} = J(x,p) + j$. We will restrict dynamics to the simultaneous level surface $(H_{\text{ext}}, J_{\text{ext}}) = 0$.

The extended 'wavefunction' $K(x,x',t,\theta)$ corresponds semiclassically to a Lagrangian manifold in P_{ext}, along with a density of pseudoparticles on that manifold, each depending parametrically on x'. The Lagrangian manifold is determined as follows. First consider the n-dimensional surface λ_0, formed by setting $x = x'$, $(t,\theta) = 0$ and $(H_{\text{ext}}, J_{\text{ext}}) = 0$. We can interpret λ_0 as a Lagrangian manifold in P. Now consider the $(n+1+k)$-dimensional surface Λ swept out in P_{ext} when the initial surface λ_0 is acted on by the set of all flows corresponding to positive t and arbitrary θ. (We only consider positive t because that is all that contributes to the integral in (3.4).) We claim that Λ is a Lagrangian manifold in P_{ext} and that the phase $W(x,x',t,\theta)$ in (3.5) is given by integrating the following 1-form on Λ

$$\Theta = p\cdot dx + h dt + j\cdot d\theta \quad (3.8)$$

with the initial condition $W = 0$ on λ_0. The assertion that λ is Lagrangian follows at once from the fact that the initial surface λ_0 is Lagrangian in P and the fact that arbitrary t- and θ-evolutions preserve both H and J. That integrating Θ gives $W(x,x',t,\theta)$ is then obvious when one notes that $h = -H(x,p)$ and $j = -J(x,p)$ on Λ. Noting that Λ is Lagrangian makes obvious our earlier assertion that the ordering of paths in (3.6) does not affect $W(x,x',t,\theta)$.

The arguments above show that the phase of (3.5) is determined by the Lagrangian manifold Λ. We next investigate the amplitude in (3.5) and interpret it in terms of a density of pseudoparticles on Λ. Good coordinates for Λ are provided by the set (p',t,θ), where, for a given point l on Λ, $p'(l)$ is the initial momentum of the (t,θ)-trajectory connecting a point $(x',p',t=0,\theta=0)$ on λ_0 to l. The amplitude in (3.5)

then comes from projecting onto coordinates (x,t,θ), the density of pseudoparticles that is given in the coordinates (p',t,θ) by the constant $(2\pi\hbar)^{-n}$

$$\begin{aligned}\varrho(x,t,\theta;x') &= \frac{1}{(2\pi\hbar)^n}\left|\frac{\partial(p',t,\theta)}{\partial(x,t,\theta)}\right| \\ &= \frac{1}{(2\pi\hbar)^n}\left|\left(\frac{\partial p'}{\partial x}\right)_{t,\theta}\right| \\ &= \frac{1}{(2\pi\hbar)^n}\left|\frac{\partial^2 W(x,x',t,\theta)}{\partial x\partial x'}\right|. \end{aligned} \tag{3.9}$$

We use here the generating function condition $p' = -\partial W/\partial x'$ on $W(x,x',t,\theta)$. The amplitude in (3.5) is obtained by taking the square root of this density, up to the phase factor $\mathrm{i}^{-n/2}$.

We can see why the amplitude should be determined by (3.9) if we note that, at $(t,\theta)=0$, the extended propagator is given by $W(x,x',0,0)=\delta(x-x')$. If we interpret this as a wavefunction in the unextended Hilbert space $\mathcal{H}$ and transform to a momentum representation, the result is a plane wave $(2\pi\hbar)^{-n/2}\exp(-\mathrm{i}p\cdot x'/\hbar)$. In terms of WKB theory, this plane wave corresponds to the Lagrangian manifold λ_0, on which there is a density of pseudoparticles given by the constant $(2\pi\hbar)^{-n}$ in coordinates p. To get the appropriate density for some other (t,θ), we then use the classical dynamics to transport this initial density along Λ in P_{ext}. The result is the density, constant in the coordinate p', that is seen in (3.9).

The full power of the preceding extended phase space picture for $K(x,x',t,\theta)$ becomes evident when we consider deriving semiclassical approximations for the reduced propagator and reduced Green's function. In deriving trace formulae, the Green's function is more relevant, so we will illustrate the details of this picture for $G_m(x,x',E)$ rather than for $K_m(x,x',t)$. The analogous calculations for $K_m(x,x',t)$ follow from rather straightforward modifications. Using the integral transform in (3.4) to compute $G_m(x,x',E)$ from $K(x,x',t,\theta)$ is equivalent, up to an overall factor, to changing from the representation (x,t,θ) to the representation (x,h,j) in the extended Hilbert space, where we identify $-j$ with $m\hbar$ and $-h$ with E. Semiclassically, this means switching from a projection of Λ and ϱ onto the representation (x,t,θ) to a projection onto the representation (x,t,j).

These observations allow us almost immediately to turn (3.5) into the following approximation for $G_m(x,x',E)$

$$\begin{aligned}G_m(x,x',E) = \frac{1}{\mathrm{i}\hbar}\frac{1}{(2\pi)^k}\frac{1}{(2\pi\mathrm{i}\hbar)^{(n-1-k)/2}}\sum_{\text{orbits}}\left|\left(\frac{\partial(p',t,\theta)}{\partial(x,E,J)}\right)_{x'}\right|^{1/2} \\ \times\exp\left(\frac{\mathrm{i}}{\hbar}S_m(x,x',E)-\mathrm{i}\frac{\nu\pi}{2}\right). \end{aligned} \tag{3.10}$$

In this approximation, the sum is taken over trajectories that start at position x' with $H=E$ and $J=m\hbar$ and end at position x after some (t,θ)-evolution. These paths correspond to the branches of Λ at the given values of (x,x',E,J). The Maslov index ν is computed from the caustics of Λ in the (x,h,j)-representation. The phase $S_m(x,x',E)$ is given by

$$S_m(x,x',E)=\int_{t-\text{path}}p\cdot\mathrm{d}x+\int_{\theta-\text{path}}p\cdot\mathrm{d}x. \tag{3.11}$$

This phase can be interpreted as an integral on Λ of the following 1-form appropriate to the (x, h, j)-representation

$$\bar{\Theta} = p \cdot \mathrm{d}x - t\mathrm{d}h - \theta \cdot \mathrm{d}j \tag{3.12}$$

where we take the initial condition $S = 0$ on λ_0. (Choosing the same initial condition for all of λ_0 makes sense because $\bar{\Theta}|_{\lambda_0} = 0$. A similar comment applies to the choice of initial condition for W.) In fact, we have $t\mathrm{d}h = 0$ and $\theta \cdot \mathrm{d}j = 0$ along (t, θ)-trajectories on Λ, so S simplifies to an integral of $p \cdot \mathrm{d}x$ when evaluated along orbits, as in (3.11).

Finally, the amplitude comes from projecting the density ϱ onto coordinates (x, h, j) as follows

$$\begin{aligned} \bar{\varrho}(x, h, j; x') &= \frac{1}{(2\pi\hbar)^n} \left| \frac{\partial(p', t, \theta)}{\partial(x, h, j)} \right| \\ &= \frac{1}{(2\pi\hbar)^n} \left| \left(\frac{\partial(p', t, \theta)}{\partial(x, E, J)} \right)_{x'} \right| \end{aligned} \tag{3.13}$$

where, in the last line, we merely switch from (h, j) to the more physical variables (H, J) and explicitly indicate that the parameter x' is being held fixed while derivatives are taken.

All of the results above can be verified directly by an explicit evaluation of the integral transform in (3.5) by means of the stationary phase approximation. Such a calculation also gives explicitly the factor $1/\mathrm{i}\hbar(2\pi)^k(2\pi\mathrm{i}\hbar)^{(n-1-k)/2}$ appearing in front of (3.10).

In section 5 we will explicitly outline how the energy levels are obtained from it through Gutzwiller-like trace formulae. We also point out that approximations for the wave functions could be obtained from the approximation with appropriate generalizations of the calculations of Bogomolny [5] or Berry [6], though space does not permit us to detail these calculations here.

4. Green's functions for rotational symmetry: a summary

In this section we compute reduced Green's functions for the case of rotational symmetry. The calculations are similar in spirit to those of section 3, so we will omit much of the detail and concentrate on the main concepts.

We will consider the case that the rotational symmetry arises through a unitary representation $R \to D(R)$ of the rotation group SO(3). We will ignore spin in this treatment, so SO(3) rather than SU(2) is the relevant symmetry group for the problem. We have in mind here the common physical case that Hilbert space $\mathcal{H} = L^2(\mathbb{R}^{3N})$ corresponds to N interacting spinless particles in 3-space and the representation $D(R)$ acts on wavefunctions according to $\psi(x_1, \ldots, x_N) \to \psi(R^{-1}x_1, \ldots, R^{-1}x_N)$. However, in practice we do not have to make any detailed assumptions about the system so we will keep the discussion general.

We begin in section 4.1 by establishing a set of notations for dealing with the rotation group and recalling those properties of it, such as the characters and invariant measure, that are necessary to compute symmetry reduced operators. Semiclassical approximations for these operators are then computed in section 4.2.

4.1. The rotation group: some notation

We begin our discussion of SO(3) with the invariant measure. The rotation group is 3-dimensional and we can parametrize elements of it by the rotation angle φ and a unit vector e along the axis of rotation. We will often write $R(e,\varphi)$. In terms of this parametrization, we can write the normalized invariant measure in the following form [9]

$$d\tilde{\mu}(R) = \frac{1}{2\pi^2}\sin^2(\varphi/2)d\Omega_e\, d\varphi \tag{4.1}$$

where $d\Omega_e$ is the solid angle surface element for the unit vector e. The coordinates (e,φ) are good coordinates everywhere on SO(3) except at the identity (though they may be double-valued, depending on what range is chosen for φ).

We will also find it convenient to use local coordinates θ that are defined in a neighbourhood of any given rotation R_0 as follows: we let $R(\theta; R_0) = \exp(\theta^a \mathcal{F}_a) R_0$, where where $\mathcal{F}_a$ are the generators for rotations about the coordinate axes of 3-space. In terms of these local coordinates, the invariant measure at the point R_0 is given by

$$d\tilde{\mu}(R_0) = \frac{1}{8\pi^2} d\theta. \tag{4.2}$$

The irreducible representations of SO(3) are labelled by the non-negative integers j, which we refer to as the angular momentum quantum numbers, and have dimension $d_j = 2j + 1$. It can be shown that the corresponding characters are given by [9]

$$\chi_j(R) = \frac{\sin\left[(j+\frac{1}{2})\varphi\right]}{\sin(\varphi/2)} \tag{4.3}$$

where φ is the angle of rotation of R.

Finally, by analogy with section 4.1, it is convenient to define the operator $V(t,R) = D(R)U(t)$ and the extended propagator $K(x,x',t,R) = \langle x|V(t,R)|x'\rangle$.

4.2. Semiclassical approximations

With the help of the information on SO(3) outlined in section 4.1, we are now ready to use (2.1) to calculate symmetry-reduced operators. In doing so, we find that the character of (4.3) is such that some of the symmetry between time evolution and group operations that was present in the calculations of the previous section is lost when one calculates the reduced Green's functions for rotational symmetry. In particular, there is less to be gained in doing the time and group integrals simultaneously in the appropriate generalization of (3.4). For this reason we go through the intermediate step in this section of calculating the reduced propagator before calculating the reduced Green's function. It is also hoped that the reduced propagator might itself be of intrinsic interest for the important case of rotational symmetry.

As before, we start with a semiclassical approximation for the extended propagator $K(x,x',t,R)$, based on a Van Vleck approximation for a non-autonomous Hamiltonian evolution. We first evolve for time t under Hamiltonian H and then use the components of angular momentum as Hamiltonians to affect the rotational part

of the evolution. If the rotation is $R(e,\varphi)$, then the rotational part of the evolution can be brought about by the Hamiltonian $\boldsymbol{J}\cdot e$, used for time φ.

The resulting approximation is

$$K(\boldsymbol{x},\boldsymbol{x}',t,R)=\frac{1}{(2\pi i\hbar)^{n/2}}\sum\left|\frac{\partial^2 W}{\partial\boldsymbol{x}\partial\boldsymbol{x}'}\right|^{1/2}\exp\left(\frac{i}{\hbar}W(\boldsymbol{x},\boldsymbol{x}',t,R)-i\frac{\mu\pi}{2}\right) \tag{4.4}$$

in which the sum is over classical trajectories that begin at $\boldsymbol{x}'$ and end at $\boldsymbol{x}$ after evolution under Hamiltonian H for time t and after a rotation R (cf. (3.5)). The phase $W(\boldsymbol{x},\boldsymbol{x}',t,R)$ is given by

$$W(\boldsymbol{x},\boldsymbol{x}',t,R)=\int_{t-\text{path}}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{x}-H\,\mathrm{d}t+\int_{R-\text{path}}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{x}-\boldsymbol{J}\cdot e\,\mathrm{d}\varphi \tag{4.5}$$

(cf. (3.6)). In appendix A we discuss the function $W(\boldsymbol{x},\boldsymbol{x}',t,R)$ in detail and show that it is naturally interpreted as the integral of a 1-form on an extended space $P\times\mathbb{R}\times\mathrm{SO}(3)$.

To calculate the reduced propagator $K_j(\boldsymbol{x},\boldsymbol{x}',t)$, we apply the operator of (2.1) to this approximation, using the information outlined in section 4.1, and compute the resulting integral over SO(3) by means of the stationary phase approximation. There are two sources of rapidly varying phase in the integral. The first and obvious one is the phase of (4.4). The second is in the character of (4.3), where we should allow for j to be of order $1/\hbar$.

To perform the stationary phase calculation, we break the character contribution $\sin\left[(j+\frac{1}{2})\varphi\right]$ into exponentials, $\exp\left[\pm i(j+\frac{1}{2})\varphi\right]$, and combine them with the exponential of (4.4). Applying the stationary phase condition to the resulting overall phase gives the conditions

$$-\frac{\partial W}{\partial\varphi}=\pm\left(j+\frac{1}{2}\right)\hbar \tag{4.6}$$

$$\frac{\partial W}{\partial e}=0. \tag{4.7}$$

In appendix A we show that the function $W(\boldsymbol{x},\boldsymbol{x}',t,R)$ obeys generating function conditions with respect to derivatives in R that allow us to reinterpret the equations above as

$$J=(j+1/2)\hbar \qquad \text{and} \qquad J-J'=0 \tag{4.8}$$

where $\boldsymbol{J}'$ and $\boldsymbol{J}$ are, respectively, the initial and final total angular momenta of the trajectory connecting $\boldsymbol{x}'$ to $\boldsymbol{x}$ and J is the magnitude of $\boldsymbol{J}$ (or $\boldsymbol{J}'$). The orbits that contribute to $K_j(\boldsymbol{x},\boldsymbol{x}',t)$ are therefore those for which the total angular momentum has magnitude $(j+\frac{1}{2})\hbar$ and the vector angular momentum is conserved, so that the rotation axis must be parallel to $\boldsymbol{J}=\boldsymbol{J}'$.

To complete the calculation, we now assume that these stationary phase points are isolated on SO(3) and compute the Gaussian stationary phase integrals about those points. We relegate the details of this calculation to appendix B and quote here the final result.

The semiclassical reduced propagator is

$$K_j(\boldsymbol{x},\boldsymbol{x}',t) \approx \frac{1}{8\pi^2}\frac{2j+1}{(2\pi \mathrm{i}\hbar)^{(n-3)/2}}\sum D_j(\boldsymbol{x},\boldsymbol{x}',t)\exp\left(\frac{\mathrm{i}}{\hbar}W_j(\boldsymbol{x},\boldsymbol{x}',t)-\mathrm{i}\frac{\mu_j\pi}{2}\right) \tag{4.9}$$

where the amplitude is given by

$$D_j(\boldsymbol{x},\boldsymbol{x}',t)=\left|\left(\frac{\partial(\boldsymbol{p}',\theta_\perp,\theta_\parallel)}{\partial(\boldsymbol{x},J_\perp-J'_\perp,J)}\right)_{\boldsymbol{x}',t}\right|^{1/2}. \tag{4.10}$$

The sum is over classical trajectories that start at $\boldsymbol{x}'$ with $J=(j+\frac{1}{2})\hbar$ and end at $\boldsymbol{x}$ after a time evolution of t and some rotation about the vector $\boldsymbol{J}$. The phase $W_j(\boldsymbol{x},\boldsymbol{x}',t)$ associated with each trajectory is given by an action integral like (4.5)

$$W_j(\boldsymbol{x},\boldsymbol{x}',t)=\int_{t-\text{path}}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{x}-H\mathrm{d}t+\int_{R-\text{path}}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{x} \tag{4.11}$$

in which the $\boldsymbol{J}\cdot\boldsymbol{e}\,\mathrm{d}\varphi$ part of the integral in (4.5) has been cancelled by the phase $(j+\frac{1}{2})\varphi$ of the character in (4.3). The Maslov index μ_j is described in appendix B. In the expression for $D_j(\boldsymbol{x},\boldsymbol{x}',t)$, the $\perp$ and $\parallel$ subscripts refer to components of vectors perpendicular and parallel respectively to the axis of rotation of the contributing trajectory. Note that the Jacobian in (4.10) brings into play trajectories near the contributing one that have slightly different endpoints $\boldsymbol{x}$ and rotations $R(\theta;R_0)$ (where R_0 is the rotation in the contributing trajectory), for which $J\neq J'$.

4.3. Semiclassical approximation for $G_j(\boldsymbol{x},\boldsymbol{x}',E)$

For computing trace formulae, we will ultimately be interested in approximating the reduced energy-dependent Green's function $G_j(\boldsymbol{x},\boldsymbol{x}',E)$. We present below the result of performing a stationary phase approximation of the one-sided Fourier transform relating $G_j(\boldsymbol{x},\boldsymbol{x}',E)$ to $K_j(\boldsymbol{x},\boldsymbol{x}',t)$ (as in (3.4)), in which we use (4.9) for the reduced propagator. The details of the calculation are not very illuminating so we do not present them. The resulting approximation is

$$G_j(\boldsymbol{x},\boldsymbol{x}',E)\approx\frac{1}{\mathrm{i}\hbar}\frac{1}{8\pi^2}\frac{2j+1}{(2\pi\mathrm{i}\hbar)^{(n-4)/2}}\sum\tilde{D}_j(\boldsymbol{x},\boldsymbol{x}',E)\exp\left(\frac{\mathrm{i}}{\hbar}S_j(\boldsymbol{x},\boldsymbol{x}',E)-\mathrm{i}\frac{\tilde{\mu}_j\pi}{2}\right) \tag{4.12}$$

where

$$\tilde{D}_j(\boldsymbol{x},\boldsymbol{x}',E)=\left|\left(\frac{\partial(\boldsymbol{p}',t,\theta_\perp,\theta_\parallel)}{\partial(\boldsymbol{x},E,J_\perp-J'_\perp,J)}\right)_{\boldsymbol{x}'}\right|^{1/2} \tag{4.13}$$

and

$$S_j(\boldsymbol{x},\boldsymbol{x}',E)=\int_{t-\text{path}}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{x}+\int_{R-\text{path}}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{x}. \tag{4.14}$$

This approximation is a sum over trajectories that begin at x' with $H = E$ and $J = (j + \frac{1}{2})\hbar$ and end at x after some time evolution, and some rotation about the direction $J = J'$. The Maslov index $\tilde{\mu}_j$ is obtained by adding 1 to μ_j if $-\partial^2 W/\partial t^2 = \partial E/\partial t$ is positive and is equal to μ_j otherwise.

It is useful to have a geometrical interpretation for the approximation (4.12) in terms of a Lagrangian manifold in P. This Lagrangian manifold $\lambda_j(x', E)$ is for fixed values of x', E and j and is formed by taking the (isotropic) initial surface $\{x = x', H = E, J = (j + \frac{1}{2})\hbar\}$ and acting on it with all possible time evolutions and acting on each individual point with all rotations about the vector J'. It is not difficult to verify that $\lambda_j(x', E)$ is indeed Lagrangian and that the phase S_j of (4.14) is obtained by integrating the 1-form $p \cdot dx$ over λ, with the condition $S_j = 0$ on the initial surface. One of the principle advantages of using this approach is that increments in the Maslov index $\tilde{\mu}_j$ can be obtained from the x-space caustics of $\lambda_j(x', E)$ in the usual way without going through the more cumbersome calculation outlined in appendix B.

5. Trace formulae

In this section, we show how the approximations for the reduced Green's functions that were derived in the previous sections may be used to derive trace formulae for symmetry-reduced spectra. The calculations here complement those of [7], where we considered trace formulae for the full spectra of systems with symmetry. Here, rather than determining all of the energy levels at once, the trace formula we consider will determine the energy levels within a symmetry class. The classical orbits contributing to this trace formula will not, as in [7], be periodic, though they will project to periodic orbits in a symmetry-reduced phase space.

The calculation proceeds by considering the trace of the reduced energy-dependent Green's function for the symmetry class j, defined as follows

$$g_j(E) \equiv \int dx\, G_j(x, x, E) = \sum_n \frac{1}{E - E_{n,j}}. \tag{5.1}$$

The reduced density of states is obtained from $g_j(E)$ in the usual way: $\rho_j(E) = -\frac{1}{\pi} \operatorname{Im} g_j(E + i0^+)$. We evaluate this integral using a stationary phase approximation.

5.1. Abelian symmetry

We illustrate some of the details for the case of Abelian symmetry, in which case we replace the symbol j by m. Let us begin by examining the stationary phase condition on the phase $S_m(x, x, E)$ of (3.11) that occurs when this approximation is applied to $G_m(x, x, E)$

$$0 = \frac{\partial S_m(x, x, E)}{\partial x} = p - p' \tag{5.3}$$

where p' and p are, respectively, the initial and final momenta of the (t, θ)-trajectory at energy E and $J = m\hbar$ that begins and ends at position x. We use here the following generating function conditions on $S_m(x, x', E)$

$$\frac{\partial S_m(x, x', E)}{\partial x} = p \qquad \text{and} \qquad \frac{\partial S_m(x, x', E)}{\partial x'} = -p' \tag{5.4}$$

which can be derived from the definition (3.11) by the usual methods. As usual, the two types of trajectories contributing in a stationary phase analysis are, closed trajectories, for which $p = p'$ and (t, θ) are finite, and so-called zero-length orbits, corresponding to the limit of trajectories for which $(t, \theta) \to 0$.

Though we do not do so here, it is possible to show [12] that the zero-length trajectories give rise the following Thomas–Fermi-like smooth density of states

$$\overline{\rho}_m(E) \approx \hbar^k \int \frac{dx\, dp}{(2\pi\hbar)^n} \delta(J - m\hbar)\, \delta(H - E). \tag{5.5}$$

The finite-length trajectories will give rise to fluctuations superimposed on this mean density and we will concentrate on these orbits in the rest of this section.

The finite-length closed orbits contributing here are not the regular periodic orbits that contribute to the full density of states, but are generalized periodic orbits in the sense that the phase space trajectory closes after some time evolution and also some non-trivial θ-evolution—we will refer to them as pseudoperiodic orbits. These orbits also arose in the calculations of [7] for the full density of states, but only through derivatives in which the θ-evolution was infinitesimal. Here, finite θ-evolutions are relevant. As in [7] we denote by (T, Θ) the values of (t, θ) necessary to close the orbit, and refer to (T, Θ) as the generalized period. The condition $\Theta = 0$ on orbits contributing to the full density of states is replaced by the condition $J = m\hbar$ for orbits contributing to the reduced density of states.

As with the regular orbits in [7], the pseudoperiodic orbits for given values of (H, J) are not isolated in phase space but occur in k-parameter families, parameterized by θ. Including time, each periodic orbit is imbedded in a $(1 + k)$-dimensional manifold, which we denote by Γ and which we parameterize with coordinates (t, θ). When computing the trace of $G_m(x, x', E)$, we will therefore need to use a degenerate stationary phase analysis around the family Γ.

To do this we introduce configuration space coordinates $x = (x_\parallel, x_\perp)$ such that the coordinate axes of the $(1 + k)$ coordinates $x_\parallel$ point along Γ and the coordinate axes of the $(n - 1 - k)$ coordinates $x_\perp$ are transverse to Γ. The integral over the $x_\perp$ coordinates can be performed using a stationary phase expansion, leaving an integral of the $x_\parallel$ coordinates over Γ as follows

$$g_m(E) = \frac{1}{i\hbar} \frac{1}{(2\pi)^k} \sum_\Gamma A(\Gamma)\, \exp\left(\frac{i}{\hbar} S_m(E) - i\frac{\sigma\pi}{2}\right) \tag{5.6}$$

where

$$A(\Gamma) = \int_\Gamma dx_\parallel \left| \left(\frac{\partial(p', t, \theta)}{\partial(x, E, J)} \right)_{x'} \right|^{1/2} \left| \frac{\partial^2 S_m(x, x, E)}{\partial x_\perp \partial x_\perp} \right|^{-1/2}. \tag{5.7}$$

The sum in (5.6) is taken over pseudoperiodic orbit manifolds Γ at energy E and $J = m\hbar$. For a given Γ, $S_m(E)$ is the action integral of (3.11), evaluated around any one of the pseudoperiodic orbits in Γ. We introduce the Maslov-index-like integer $\sigma = \nu + \tau$, where τ is the number of negative eigenvalues of the $(n-1-k)\times(n-1-k)$ matrix $\partial^2 S_m(x, x, E)/\partial x_\perp \partial x_\perp$.

The main thrust of the calculation will be to give $A(\Gamma)$ a more transparent, intrinsic interpretation than is evident in (5.7). As a first step, we expand the matrix

$\partial^2 S_m(x,x,E)/\partial x_\perp \partial x_\perp$ according to the chain rule and reinterpret its determinant as a Jacobian

$$\begin{aligned}\frac{\partial^2 S_m(x,x,E)}{\partial x_\perp \partial x_\perp} &= \frac{\partial^2 S_m(x,x',E)}{\partial x_\perp \partial x_\perp} + \frac{\partial^2 S_m(x,x',E)}{\partial x_\perp \partial x'_\perp} + \frac{\partial^2 S_m(x,x',E)}{\partial x'_\perp \partial x_\perp} \\ &\quad + \frac{\partial^2 S_m(x,x',E)}{\partial x'_\perp \partial x'_\perp} \\ &= \left(\frac{\partial(p_\perp - p'_\perp)}{\partial x_\perp}\right)_{x'_\perp} + \left(\frac{\partial(p_\perp - p'_\perp)}{\partial x'_\perp}\right)_{x_\perp} \\ &= 2\left(\frac{\partial(p_\perp - p'_\perp)}{\partial(x_\perp + x'_\perp)}\right)_{x_\perp - x'_\perp, x_\parallel, x'_\parallel, E, J} \\ &\sim \left(\frac{\partial(p_\perp - p'_\perp, x_\perp - x'_\perp)}{\partial(x_\perp, x'_\perp)}\right)_{x_\parallel, x'_\parallel, E, J} \\ &\sim \frac{\partial(z_\perp - z'_\perp, x_\parallel, x'_\parallel, E, J)}{\partial(x, x', E, J)} \end{aligned} \tag{5.8}$$

where $\sim$ stands for 'has the same determinant as, up to a sign'. The quantities $p_\parallel$, $p_\perp$, $z_\parallel$ and $z_\perp$ represent a seperation of phase space variables according to the decomposition $x = (x_\parallel, x_\perp)$. All derivatives above are taken at constant $x_\parallel$, $x'_\parallel$, E and J, except in the last line where we explicitly indicate otherwise. Also, we set $x = x'$ and $p = p'$ *after* all derivatives have been taken.

Using (5.8) and the chain rule, we can combine the two factors in the integrand of (5.7) to give the following form for $A(\Gamma)$

$$A(\Gamma) = \int_\Gamma \mathrm{d}x_\parallel \left|\frac{\partial(z_\perp - z'_\perp, x_\parallel, x'_\parallel, E, J)}{\partial(z'_\perp, z'_\parallel, t, \theta)}\right|^{-1/2}. \tag{5.9}$$

The next step is to eliminate $\mathrm{d}x_\parallel$ in favour of the natural volume element $\mathrm{d}t\,\mathrm{d}\theta$ on Γ. We do this by using the chain rule to seperate out an appropriate Jacobian from the integrand of (5.9) and combining with $\mathrm{d}x_\parallel$ as follows

$$\mathrm{d}x_\parallel \left|\frac{\partial(z'_\perp, x_\parallel, x'_\parallel, E, J)}{\partial(z'_\perp, z'_\parallel, t, \theta)}\right|^{-1/2} = \mathrm{d}t\,\mathrm{d}\theta. \tag{5.10}$$

This identity was shown under similar conditions in [7], so we refer the reader there for details.

We are left with the following expression for $A(\Gamma)$

$$A(\Gamma) = \int_\Gamma \mathrm{d}t\,\mathrm{d}\theta \left|\left(\frac{\partial(z_\perp - z'_\perp)}{\partial z'_\perp}\right)_{x_\parallel, x'_\parallel, E, J}\right|^{-1/2}. \tag{5.11}$$

The Jacobian in the integrand here also turned up in [7], where we found that it was related to a linearization M of a reduced surface of section map as follows

$$\left|\left(\frac{\partial(z_\perp - z'_\perp)}{\partial z'_\perp}\right)_{x_\parallel, x'_\parallel, E, J}\right| = |\det(M - I)|. \tag{5.12}$$

The surface of section Σ is formed by setting $H = E$, $J = m\hbar$ and fixing $x_\parallel$. The map $\psi : \Sigma \to \Sigma$ is obtained by starting trajectories on Σ near Γ, letting them flow once around Γ, and finally using the $1 + k$ flow parameters (t, θ) to get trajectories back onto Σ.

We are just left with a normalization of the volume element $\mathrm{d}t\,\mathrm{d}\theta$ over Γ, which we denote by

$$W_0 = \int_\Gamma \mathrm{d}t\,\mathrm{d}\theta. \tag{5.13}$$

W_0 is equivalent to the quantity $T_0 V_0$ that was introduced in [7], where T_0 is the period of a primitive periodic orbit and V_0 represents the θ part of the integral over Γ. We have changed notation because the definition of the primitive period T_0 is somewhat ambiguous when θ-evolutions are allowed in closing the orbit.

The final result is the following trace formula for $g_m(E)$ in terms of generalized periodic orbits

$$g_m(E) \approx \frac{1}{\mathrm{i}\hbar}\frac{1}{(2\pi)^k}\sum_\Gamma \frac{W_0}{|\det(M - I)|^{1/2}} \exp\left(\frac{\mathrm{i}}{\hbar}S_m(E) - \mathrm{i}\frac{\sigma\pi}{2}\right). \tag{5.14}$$

The reader will notice that this trace formula is remarkably like the regular trace formula of Gutzwiller, applied to the isolated periodic orbits of the symmetry-reduced classical dynamics. We will explore this question in the next section. First, however, let us review the various quantities contributing to (5.14).

The sum is taken over orbits that close in phase space after a (t, θ)-evolution of (T, Θ), at energy $H = E$ and $J = m\hbar$. The phase $S_m(E)$ occurring in the contribution of each orbit is an integral of $p \cdot \mathrm{d}x$ around both the t and θ parts of the orbit, as in (3.11).

While we do not do so here, it is possible to show [12] that σ is the Maslov index of the stable or unstable manifold of the periodic orbit family Γ. This interpretation is possible because the invariant manifolds are Lagrangian for the Abelian symmetries considered in this section, and therefore they have well-defined Maslov indices. This result generalizes the results of [13, 14] for the Maslov index of the regular trace formula.

In the amplitude term, W_0 is the normalization of the volume element $\mathrm{d}t\,\mathrm{d}\theta$ on Γ. This is often just $(2\pi)^k T_0$, where T_0 is the time period of the first repetition of the orbit, however this is not always the case, as we discuss in the next section. The $2(n - 1 - k) \times 2(n - 1 - k)$ matrix M is a linearization of a reduced surface of section mapping, whose construction was described in detail in [7]. We can also use a linearization of a regular surface of section mapping constructed for the classically reduced dynamics.

The trace formulae [7] for the full density of states can be recovered in the case of Abelian symmetry by summing over the partial densities in (5.14) and using a

stationary phase approximation. The stationary phase contributions come from those families Γ' of orbits which $\Theta = 0$, and the result is a sum over families Γ' like (5.14) except for two structural differences. The first is that a square root of the determinant of the $k \times k$ symmetric matrix $\partial\Theta/\partial J = \partial^2 S/\partial J \partial J$ appears in the denominator and the second is that the Maslov index must be replaced by $\sigma' = \sigma + \delta$, where δ is the number of positive eigenvalues of $\partial\Theta/\partial J$. (These results were derived in [12].)

An important special case of the systems considered in this section is when $k = n - 1$, so that there are enough first integrals to make the system integrable. In this case the Γs correspond to the discrete set of invariant tori specified by $H = E$ and $J = (j + \frac{1}{2})\hbar$, and the sum in (5.14) reduces to a sum over iterations of corresponding primitive orbits. Just as in the case of the regular Gutzwiller sum applied to 1-dimensional systems, this can be summed geometrically. The result is equivalent to the well-known torus or EBK quantization conditions. Details of this straightforward calculation can be found in [12]. Along with the demonstration that the sum in (5.15) for the full density of states can be decomposed into the partial sums of (5.14), this calculation shows in a very transparent way the fact that the Gutzwiller sum is equivalent to torus quantization (cf. [15]).

5.2. Rotational symmetry

One finds a similar trace formula for the case of rotational symmetry by tracing over (4.12). In this section we present the results of such a calculation.

The interesting stationary phase contributions to the trace of $G_j(\boldsymbol{x}, \boldsymbol{x}', E)$ come from orbits with $H = E$ and $J = (j + \frac{1}{2})\hbar$ that close after some time evolution (time T say) and some rotation R. Because J must return to its original value at the end of the orbit, R must be a rotation about the direction of J, and we denote by $\Theta_{\|}$ the angle of rotation about this axis. By acting on the initial point of any orbit by arbitrary time evolutions and rotations, we map out a 4-dimensional surface Γ in phase space, consisting of points that are periodic under a time evolution of T and a rotation through angle $\Theta_{\|}$ about the angular momentum direction.

Just as in (5.6), the result of a degenerate stationary phase analysis is a sum over families of orbits Γ, with the contribution of each family being determined by a 4-dimensional volume integral over that family. We will not provide the details of the analysis of that volume integral here, but we will give a detailed description of the results. A full and explicit analysis can be found in [12].

The result of the analysis is

$$g_j(E) \approx \frac{2j+1}{i\hbar} \sum_{\Gamma} \frac{W_0}{|\det(M - I)|^{1/2}} \exp\left(\frac{i}{\hbar} S_j(E) - i\frac{\sigma\pi}{2}\right). \quad (5.15)$$

In the phase, $S_j(E)$ is an action integral around any one of the orbits on Γ, including the rotational part of the orbit, and σ is a Maslov index.

In the amplitude, W_0 represents an integral of the natural volume element $\mathrm{d}t\,\mathrm{d}\tilde{\mu}(R)$ over Γ

$$W_0 = \int_{\Gamma} \mathrm{d}t\,\mathrm{d}\tilde{\mu}(R). \quad (5.16)$$

W_0 can also be interpreted on a reduced phase space as the period of an appropriately defined primitive periodic orbit, as discussed in section 6. Also in the amplitude, M

is the linearization of a certain symmetry-reduced surface of section map, discussed in detail in [7]. We review briefly here the construction of this map.

The constructions of the reduced surface of section Σ and the associated map ψ are similar to the analogous constructions of section 5.1 for Abelian symmetry, except that there are modifications to take into account the fact that only the magnitude J and not the full vector J of first integrals is conserved by all symmetries. To form Σ we set $H = E$ and $J = (j + \frac{1}{2})\hbar$, and fix any other 4 independent functions such that the resulting $2(n-3)$-dimensional surface Σ intersects Γ at a point. The map ψ is formed by taking trajectories that start on Σ around Γ and using the 4 independent parameters of evolution (t, R) to make those trajectories return to Σ. As discussed in [7], this map is symplectic and has no remaining symmetry. As discussed in the next section, this map is closely related to a regular surface of section maps on a reduced phase space. M is the linearization of ψ at Γ.

It should be noted that this discussion of (5.15) does not hold in the important special case $j = 0$. The trace formula in that case is still formally like (5.15) applied to orbits with $H = E$ and $J = 0$, except for two differences which reflect the fact that the classical reduction procedure is special for $J = 0$ (proved in [12]). The reduction procedure is different in this case because setting $J = 0$ is equivalent to setting all three components of J to 0, which results in one fewer degrees of freedom for the reduced system. For example, following the procedures outlined in this paper, the reduced surface of section Σ has dimension $2(n-4)$ rather than $2(n-3)$. The first difference therefore is that the linearized map M has dimension $2(n-4)$ instead of $2(n-3)$. The second difference is that the factor $(2\pi i\hbar)^{-(n-3)/2}$ should be replaced with $(2\pi i\hbar)^{-(n-4)/2}$.

We should also note that the results of [7] for rotational symmetry are recovered by summing over j in a stationary phase approximation. The result is a sum like (5.15) and the details are presented in [12].

Finally, we remark that that the form of (5.15) is easily applied to general symmetries if the degeneracy factor $2j + 1$ is replaced by the dimension d_j of a general irreducible representation. Of course, points on Γ are now parametrized by (t, g) and the appropriate volume element with which to compute W_0 is $\mathrm{d}t\,\mathrm{d}\tilde{\mu}(g)$ where $\mathrm{d}\tilde{\mu}(g)$ is the normalized invariant measure for the general symmetry group G. However, we have not shown that this extension is valid and leave it as a (rather natural) conjecture.

6. Connection with Gutzwiller's sum for non-symmetric systems

The forms of (5.14) and (5.15) are very reminiscent of the regular trace formula, except that the periodic orbit sum is applied to the periodic orbits of a symmetry-reduced classical phase space rather than full phase space. In this section, we will explore this connection further, and we will show that the identification is largely correct. In doing so however, some of the seemingly obvious correspondences between the trace formulae of section 6 and the usual formula for non-symmetric systems exhibit somewhat subtle complications, and we will examine these in detail.

The most obvious point to make is that the families of pseudoperiodic orbits contributing to the sums in (5.14) and (5.15) correspond to regular periodic orbits in a symmetry-reduced classical phase space (figure 1). For notational purposes, it is convenient to first explain this in the most interesting case of rotational symmetry—with minor modifications that we outline at the end of the section, the discussion

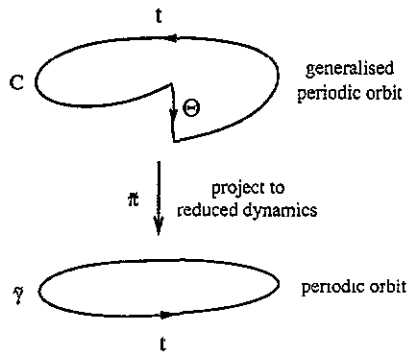

Figure 1. On passing from the full dynamics to the symmetry-reduced dynamics, a pseudoperiodic orbit (C) projects to a regular periodic orbit in reduced phase space.

can easily be applied to other symmetries. We first give a brief description of the classical reduction process. The discussion follows the general theory, described in Arnol'd [16], and more fully in Abraham and Marsden [17].

Given a classical system with rotational symmetry, the first step is to restrict dynamics to a level surface $\mathcal{E}_J$ of the magnitude J of total angular momentum. Notice that this surface is invariant under time evolution and also arbitrary rotations. Therefore, the full group SO(3) is a symmetry group of this restricted dynamical system. The reduced phase space $\tilde{P}_J$ is then formed by identifying, in this restricted space, points that are related to each other by some symmetry transformation. Technically, the reduced phase space is the quotient space $\tilde{P}_J = \mathcal{E}_J/\mathrm{SO}(3)$. We denote by π the projection from $\mathcal{E}_J$ to $\tilde{P}_J$. Notice that forming the quotient space here is analogous to ignoring the θ coordinate in the case of axial symmetry and that the restriction of dynamics to $\mathcal{E}_J$ is analogous to fixing p_θ to some constant value in that case.

Trajectories on reduced phase space are obtained by projecting down to $\tilde{P}_J$ trajectories on $\mathcal{E}_J$. This defines a well-defined set of dynamics on $\tilde{P}_J$ because trajectories on $\mathcal{E}_J$ display SO(3)-symmetry. It is evident that a pseudoperiodic orbit family Γ at $J = (j+\frac{1}{2})\hbar$ projects down to a regular periodic orbit $\tilde{\gamma}$ in $\tilde{P}_j$ (where, in a slight change of rotation, we label the reduced phase space by the integer j rather than J). Therefore (5.15) can be interpreted as a sum over the periodic orbits of energy E in the reduced system, and these are isolated if SO(3) is the only symmetry of the original system.

Perhaps the most important feature of the periodic orbit sum is the phase variation $S_j(E)$, and to interpret this we must examine the symplectic structure of $\tilde{P}_j$. We define a sympectic form $\tilde{\Omega}$, acting on two vectors $\tilde{u}$ and $\tilde{v}$ tangent to $\tilde{P}_j$, as follows. We find two vectors u and v tangent to $\mathcal{E}_J$, for which $\tilde{u} = \pi_* u$ and $\tilde{v} = \pi_* v$, and define $\tilde{\Omega}(\tilde{u},\tilde{v}) = \Omega(u,v) - J_a \epsilon^{abc} \mathrm{d}J_b(u)\mathrm{d}J_c(v)$, which turns out [17], to be independent of the choice of u and v.

While the symplectic form can naturally be projected down to $\tilde{P}_j$ in this way, the same is not true for the 1-form $\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{x}$ with which $S_j(E)$ is calculated. This causes considerable problems in interpreting the trace formula entirely in terms of reduced phase space. To examine $S_j(E)$, let us associate with the pseudoperiodic orbit a definite path C in phase space, obtained by first applying time-evolution for time T to some initial point on Γ, and then applying the rotation through angle $\Theta_{\|}$ about the direction of $\boldsymbol{J}$. $S_j(E)$ is then the integral of $\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{x}$ around C.

Let us initially suppose that it is possible to find a 2-dimensional surface $\mathcal{R}$ on

which J is constant (actually, it is necessary only to assume that J be constant on $\mathcal{R}$, but the stronger assumption simplifies the argument considerably) and which is bounded by C in such a way that $C = -\partial\mathcal{R}$. Then Stokes' theorem tells us that $S_j(E)$ is obtained by integrating the full phase space symplectic form Ω over $\mathcal{R}$ as follows

$$S_j(E) = \int_{\mathcal{R}} \Omega. \tag{6.1}$$

Now we note that the curve C projects to the periodic orbit $\tilde{\gamma}$ in reduced phase space and $\mathcal{R}$ projects to a surface $\tilde{\mathcal{R}}$ bounded by $\tilde{\gamma}$. We can immediately write

$$S_j(E) = \int_{\mathcal{R}} \Omega = \int_{\mathcal{R}} \tilde{\pi}^* \tilde{\Omega} = \int_{\tilde{\pi}_* \mathcal{R}} \tilde{\Omega} = \int_{\tilde{\mathcal{R}}} \tilde{\Omega} \tag{6.2}$$

where we use the fact that $\mathrm{d}J = 0$ on $\mathcal{R}$. Therefore it is possible in this case to associate $S_j(E)$ with an action of $\tilde{\gamma}$ defined entirely within reduced phase space.

It is not always possible, however, to find a surface $\mathcal{R}$ for which the stated conditions hold, and in this case (6.2) is not valid. It is simplest to illustrate such an exception with the case of axial symmetry in 3-degrees of freedom rather than with rotational symmetry. The reduction process is the same except that J is replaced with J_z and SO(3) is replaced with SO(2). We consider in particular the case of a curve C which encircles the z-axis and for which $J_z \neq 0$. Then any surface which is bounded by C must intersect the z-axis in configuration space, and this is incompatible with the condition that $J_z = xp_y - yp_x \neq 0$. We expect similar exceptions to occur for more complicated systems.

The topological problems outlined above in using $\tilde{\Omega}$ to compute $S_j(E)$ presents a serious problem because, as mentioned previously, it is not always possible to define a global 1-form on $\tilde{P}_j$ in a natural way. An example for which this can be seen is that of a free rigid body (a spherically symmetric system), for which the reduced phase space is topologically a sphere and the reduced symplectic form is proportional to the solid angle 2-form, ω say [8]. It is not difficult to see that there is no globally-defined 1-form θ for which $\omega = -\mathrm{d}\theta$. Similar considerations hold for N-body systems with overall spherical symmetry.

Of course, it is sometimes possible in specific examples to overcome these problems. (For example, in the case of an axially symmetric 3-degree-of-freedom system, one can define a 1-form $p_\rho \mathrm{d}\rho + p_z \mathrm{d}z$ on the reduced space. It can be shown that integrating this around reduced periodic orbits gives a result which differs from $S_m(E)$ by a term $2\pi N J_z$, where the integer N is the winding number of the orbit C around the z-axis. When $J_z = m\hbar$, this term does not affect the periodic orbit sum.) However, it is not clear that there is an easy interpretation for $S_j(E)$ in terms of $\tilde{P}_j$ that is applicable with complete generality. For this reason, we believe that the full phase space definition as an integral of $\boldsymbol{p} \cdot \mathrm{d}\boldsymbol{x}$ around C remains the conceptually most useful interpretation for $S_j(E)$.

The factor W_0 also needs consideration. For a given orbit with generalized period $(T, \Theta_{\|})$, let $\tilde{T}_0$ be the primitive period of the corresponding orbit $\tilde{\gamma}$ in reduced phase space. We can then parametrize points in Γ with a time coordinate t between 0 and $\tilde{T}_0$ and rotations R in SO(3). If, for a given t, every different R corresponds to a distinct point on Γ, then the integral in (5.16) defining W_0 breaks into a time integral giving $\tilde{T}_0$, and an integral of the normalized invariant measure over SO(3), giving 1.

It is possible, however, that a given point on Γ has a discrete isotropy subgroup of N_I rotations that leave the point invariant. In this case a point on Γ will correspond to N_I rotations in SO(3) and the estimate above for W_0 overcounts by a factor of N_I. Instead we must use

$$W_0 = \frac{\tilde{T}_0}{N_I}. \tag{6.3}$$

This effect of the discrete symmetry is counteracted, however, by the fact that N_I different orbits corresponding to the same reduced orbit $\tilde{\gamma}$ will contribute to the sum in (5.15), each giving the same contribution. If $\Theta_{\|_i}$ with $1 \leqslant i \leqslant N_I$ are the rotation angles of the elements of the symmetry group, and $(T, \Theta_\|)$ is the generalized period of an orbit on Γ, then there are associated with this orbit N_I generalized periodic orbits with generalized period of the form $(t, \Theta_\| + \Theta_{\|_i})$. Even though each of these orbits corresponds to the same manifold of points in phase space, each contributes separately in (5.15), just as multiple repetitions of a primitive orbit contribute separately to Gutzwiller's sum. Each of these orbits projects to the same reduced orbit $\tilde{\gamma}$ and gives an identical contribution to (5.15).

The effect is that if we just sum over reduced orbits $\tilde{\gamma}$, we can replace (5.15) with a sum that is identical in form to the regular Gutzwiller sum applied to the periodic orbits of the reduced dynamics

$$g_j(E) \approx \frac{1}{i\hbar} \sum_{\tilde{\gamma}} \frac{\tilde{T}_0}{|\det(M - I)|^{1/2}} \exp\left(\frac{i}{\hbar} S_j(E) - i\frac{\sigma\pi}{2}\right). \tag{6.4}$$

Thus we arrive at the pleasing result that the quantally reduced spectrum is determined by the classically reduced periodic orbits in the usual way.

We point out that this discussion can be modified for the case of Abelian symmetry by some easy modifications. The reduced phase space is formed by fixing the full set of constants $\boldsymbol{J}$ and modding out by the symmetry group. The appropriate reduced phase spaces for the reduced trace formulae are then labelled by the integer vectors $\boldsymbol{m}$, for which $\boldsymbol{J} = \boldsymbol{m}\hbar$. The discussion can then be generalized almost as simply as replacing j with $\boldsymbol{m}$ everywhere in the argument.

7. Conclusion

We have seen in this paper that the symmetry-projected propagators and Green's functions of a system with continuous symmetry can be approximated in terms of classical trajectories that are the result of both time evolution and the application of some symmetry operation. In return for allowing symmetry operations as well as time evolution, the trajectories are constrained to certain values of the first integrals that are implied by the symmetry. These values correspond to the irreducible representation that one is interested in (e.g. $J = (j + 1/2)\hbar$ for rotational symmetry). The results in this paper are consistent in form with the previous work of Robbins [11] on the case of discrete symmetry.

The process of allowing symmetry operations but restricting the first integrals, as in $J = (j + 1/2)\hbar$ for rotational symmetry, corresponds precisely to looking at orbits in a symmetry-reduced classical phase space. That is, we find that restricting operators,

wavefunctions etc. to a subspace of Hilbert space corresponding to a given irreducible representation goes over in the classical limit to the classical reduction process of fixing the first integrals and then quotienting out by the symmetry group [16, 17]. Many of the classical structures that arose in the calculation, for example the Lagrangian manifolds from which the phases of the Green's functions are constructed, project naturally to symmetry-reduced classical phase space (this point is discussed more fully in [12]). Therefore, in some loose sense, we can think of the semiclassical Green's functions as being determined by the classically reduced phase spaces. There are problems in interpreting this analogy in a precise way however because the classical reduced phase space does not necessarily decompose naturally into configuration and momentum spaces. Therefore we cannot, for example, write the Green's functions in terms of an argument $(\overline{x}, \overline{x}')$, consisting of configuration space coordinates on reduced phase space, or find a natural counterpart in reduced phase space to the 1-form $p \cdot \mathrm{d}x$ that determines the phase. Nevertheless, any structures that depend purely on symplectic geometry can be naturally restricted to the reduced space, so in a purely formal sense, the natural classical limit of the restricted Hilbert space $\mathcal{H}_j$ is reduced phase space.

As well as approximations for the Green's functions themselves, we computed their traces and found Gutzwiller-type trace formulae for the symmetry-projected densities of states. These trace formulae involve families of orbits that close on themselves after time evolution and a symmetry operation (which we called pseudoperiodic orbits). These orbits correspond to regular periodic orbits in the dynamics of reduced phase space so the trace formulae, like the Green's functions, can be interpreted formally as depending on the classically reduced phase space. In fact, we showed in section 6 that the symmetry-projected trace formula looks exactly like the regular Gutzwiller formula applied to the dynamics of reduced phase space. However, the actions and Maslov indices ocurring in these formulae are unambiguously determined only by the full phase space structures.

The derivations presented in this paper were for the particular cases of continuous Abelian and rotational symmetry. These cases, epecially rotational symmetry, are very important physically, and it is expected that the results presented here will be of use in nuclear, atomic or molecular problems where rotational symmetry is an important factor. The final results do not, however, depend in an obvious way on the particular type of symmetry, so we expect that they can be applied without significant modification to systems with arbitrary symmetry, as outlined at the end of section 5. We have not, however, proved this.

Appendix A

In this appendix we use an extended phase space $\mathcal{P} = P \times \mathbb{R} \times \mathrm{SO}(3)$ to investigate the function $W(x, x', t, R)$, and in particular to justify the generating function conditions that lead to (4.6) and (4.7) (see also (B2)).

First of all, let λ_0 be any Lagrangian manifold in regular phase space P. We will ultimately let λ_0 be specified by the conditions $x = x'$, but for now we let it be arbitrary. If we act on λ_0 with all possible rotations and time evolutions, we generate a $(n + 1 + k)$-dimensional manifold Λ in $\mathcal{P}$ and we claim that the following 1-form is closed on Λ

$$\Theta = p \cdot \mathrm{d}x - H\mathrm{d}t - J_a \omega^a. \tag{A1}$$

Here, the 1-forms ω^a are to be interpreted as 1-forms on SO(3) that are obtained by right translating the three basis vectors of so(3)*, the dual to the Lie algebra so(3). The 1-form ω^a, acting on any given vector tangent to SO(3), gives the ath component of the vector relative to the local coordinates θ. We point out that $\mathrm{d}\omega^a \neq 0$

Taking the differential of Θ we find

$$-\mathrm{d}\Theta = \Omega - \mathrm{d}t \wedge \mathrm{d}H - \omega^a \wedge \mathrm{d}J_a + J_a \mathrm{d}\omega^a \tag{A2}$$

where Ω is the usual symplectic form on phase space. Using the fact that λ_0 is Lagrangian and the fact that [17] $\mathrm{d}\omega^a(Y_\xi, Y_\eta) = \langle \omega^a, Y_{[\xi,\eta]} \rangle$, where Y_ξ is the right invariant vector field on SO(3) associated with the Lie algebra element ξ, it is not difficult to show [12] that $\mathrm{d}\Theta|_\Lambda = 0$. We do not show the details here however.

Now choose λ_0 to be the initial Lagrangian manifold $x = x'$ and define the function W to be the integral of Θ on Λ, which is path-independent because $\mathrm{d}\Theta|_\Lambda = 0$. This definition of W is easily seen to coincide with the definition of (4.5) and from the form of Θ in (A1) we can immediately write down the following relationships

$$\frac{\partial W(x, x', t, R)}{\partial \theta^a} = -J_a. \tag{A3}$$

To derive the relationships in (B2) we must relate the coordinates θ to the coordinates $(\psi, \theta_\parallel)$ (defined in appendix B) and this is done in appendix C. We use (C1) proved there to see that

$$-\frac{\partial W}{\partial \psi} = -\frac{\partial W}{\partial \theta} \cdot \frac{\partial \theta}{\partial \psi} = (I - \tilde{R}_0)J = J - J' \tag{A4}$$

$$-\frac{\partial W}{\partial \varphi} = -\frac{\partial W}{\partial \theta} \cdot \frac{\partial \theta}{\partial \varphi} = e_0 \cdot J \tag{A5}$$

where we use $\tilde{R}_0 J = R_0^{-1} J = J'$. Also, in (A5), we take only the two components perpendicular to e_0.

Appendix B

In this appendix, we supply the missing details of the calculation in section 4 leading up to (4.9).

First, in order to understand more fully the stationary phase conditions (4.8), and in order to facilitate the coming stationary phase calculation, we introduce a parametrization of unit vectors e near the zero-order unit vector e_0 by coordinates ψ, which are defined approximately through

$$e \approx e_0 + \psi \times e_0. \tag{B1}$$

We can think of ψ as a 2-vector in the plane perpendicular to e_0 and we can define this vector more precisely through $e = \exp(\psi^a \mathcal{F}_a) e_0$. It is not difficult to see that at e_0 the solid-angle surface element can be expressed in the form $\mathrm{d}\Omega_{e_0} = \mathrm{d}\psi$. We can now use the local variables (ψ, φ) rather than (e, φ) to parametrize rotations.

If we expand $W(x, x', t, R)$ around an orbit for which $J = Je_0$, we can derive the following generating function conditions

$$-\frac{\partial W}{\partial \varphi} = J \cdot e_0 = J \qquad \text{and} \qquad -\frac{\partial W}{\partial \psi} = J - J' \tag{B2}$$

which are easily seen to imply (4.8). (B2) is a generalization of the condition $\partial W/\partial t = -H$ satisfied by the ordinary Hamilton's principal function and is derived in appendix A.

To complete the stationary phase approximation of the integral over SO(3) for $K_j(x, x', t)$, we expand the phase $W(x, x', t, R)$ out to second order in the variables (φ, ψ) and evaluate the resulting 3-dimensional Gaussian integral. With the help of (B2), the Hessian matrix which determines the quadratic phase can be manipulated in the following way

$$-\begin{pmatrix} \frac{\partial^2 W}{\partial \psi \partial \psi} & \frac{\partial^2 W}{\partial \varphi \partial \psi} \\ \frac{\partial^2 W}{\partial \psi \partial \varphi} & \frac{\partial^2 W}{\partial \varphi \partial \varphi} \end{pmatrix} = \begin{pmatrix} \frac{\partial (J - J')}{\partial \psi} & \frac{\partial (J - J')}{\partial \varphi} \\ \frac{\partial e \cdot J}{\partial \psi} & \frac{\partial e \cdot J}{\partial \varphi} \end{pmatrix}$$

$$\sim \frac{\partial (J - J', e \cdot J)}{\partial (\psi, \varphi)} \tag{B3}$$

where, as usual, the symbol $\sim$ indicates that the determinants are the same up to a sign. In all the derivatives here, x, x' and t are held fixed. Also, $J - J'$ and ψ are to be interpreted as 2-vectors in the plane orthogonal to e. In order to emphasize that only the two components of $J - J'$ perpendicular to e are relevant in this Jacobian, we will in future write $J_\perp - J'_\perp$. Finally, because variations in J coincide with those in $e \cdot J$ to first order, it is legitimate to replace $e \cdot J$ with J in the last line of (B3).

Computing the Gaussian integral then results in the approximation for $K_j(x, x', t)$ that we see in (4.9), with the amplitude $D_j(x, x', t)$ given by the following equation

$$D_j(x, x', t) = \left| 4 \sin^2(\varphi/2) \left(\frac{\partial (p', \psi, \varphi)}{\partial (x, J_\perp - J'_\perp, J)} \right)_{x', t} \right|^{1/2}. \tag{B4}$$

To get this we have already used the chain rule to combine the Jacobian of (B3) with the amplitude in (4.4). We can simplify the form of (B4) further by using the local coordinates θ (whose construction is discussed in the paragraph preceding (4.2)) instead of (ψ, φ). To do this we note that the two sets of coordinates on SO(3) are related through the Jacobian

$$\left| \frac{\partial (\theta_\perp, \theta_\parallel)}{\partial (\psi, \varphi)} \right| = 4 \sin^2(\varphi/2) \tag{B5}$$

where, for the sake of symmetry, we split θ into a single component $\theta_\parallel$ parallel to e and two components $\theta_\perp$ perpendicular to e. (B5) is proved in appendix C. Using this relationship, we can rewrite the amplitude $D_j(x, x', t)$ in the form given in (4.10).

Let us finally outline how the Maslov index μ_j is determined in these calculations. The Maslov index μ_j receives contributions from a number of different sources which we outline as follows. The first contribution is from the Maslov index μ of the propagator $K(x, x', t, R)$. To this we must add the number of positive eigenvalues of the symmetric Hessian matrix in (B3) (notice that there is a minus sign in front of this matrix). Then, if $\sin(\varphi/2)$ is negative, we must add 2 to the index to account for absorbing the $\sin(\varphi/2)$ term inside the modulus of (B4). We decide on a definite angle φ by choosing the sign of e such that $e \cdot J > 0$ and choosing φ to lie between $-\pi$ and π. With this choice of φ, it is the $\exp\left[+\mathrm{i}(j+\frac{1}{2})\varphi\right]/2\mathrm{i}$ part of the $\sin\left[(j+\frac{1}{2})\varphi\right]$ term that gives rise to the stationary phase condition in (4.6) and (4.7). Finally, we add 1 to the index to account for the phase factor of $1/\mathrm{i}$ that arises when $\sin\left[(j+\frac{1}{2})\varphi\right]$, is broken into exponentials.

Appendix C

In this appendix we consider the relationship between the local coordinates $(\theta_\perp, \theta_\parallel)$ and (ψ, φ), and show that the Jacobian corresponding to a change from one set of these coordinates to the other is given by (B5).

Let us consider these sets of coordinates in the neighbourhood of some definite rotation $R_0 = R(e_0, \varphi_0)$. We prove (B5) by showing that, to first order in small variations away from R_0

$$\theta_\parallel = \varphi - \varphi_0 \qquad \text{and} \qquad \theta_\perp = \psi - R_0\psi. \tag{C1}$$

We can then express the Jacobian for the change of coordinates $(\psi, \varphi) \to (\theta_\perp, \theta_\parallel)$ in the form

$$\begin{aligned}\left|\frac{\partial(\theta_\perp, \theta_\parallel)}{\partial(\psi, \varphi)}\right| &= \begin{vmatrix} (I - R_0)_\perp & 0 \\ 0 & 1 \end{vmatrix} \\ &= \left|(1 - \mathrm{e}^{\mathrm{i}\varphi_0})(1 - \mathrm{e}^{-\mathrm{i}\varphi_0})\right| \\ &= 4\sin^2(\varphi_0/2)\end{aligned} \tag{C2}$$

where by $(I - R_0)_\perp$ we mean the restriction of the matrix $I - R_0$ to the plane perpendicular to e_0. This last form reproduces exactly (B5).

In order to justify (C1), we let $\mathcal{R}(\theta)$ and $\mathcal{R}(\psi)$ represent the near-identity rotations corresponding to the vectors θ and ψ respectively, and note that the definitions of these coordinates allow us to write

$$\begin{aligned}&\mathcal{R}(\theta)R_0 = R(\mathcal{R}(\psi)e_0, \varphi) = \mathcal{R}(\psi)R(e_0, \varphi - \varphi_0)R_0\mathcal{R}(\psi)^{-1} \\ \Rightarrow\ &\mathcal{R}(\theta) = \mathcal{R}(\psi)R(e_0, \varphi - \varphi_0)R_0\mathcal{R}(\psi)^{-1}R_0^{-1} \\ &= \mathcal{R}(\psi)R(e_0, \varphi - \varphi_0)\mathcal{R}(R_0\psi)^{-1}.\end{aligned} \tag{C3}$$

Each of the three matrices in this last form is near-identity, so we can expand out the matrices to first order in terms of 3-vectors. Doing so, and equating components with those on the left hand side, we immediately recover (C1).

Acknowledgments

I would like to thank R G Littlejohn for much helpful input in this work and in previous collaborations. I would also like to thank Jim Morehead for many useful discussions and for careful reading of the manuscript. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, of the US Department of Energy under contract No DE-AC03-76SF00098, and by the National Science Foundation under Grant No NSF-PYI-84-51276.

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