Semiclassics of rotation and torsion

Petr A. Braun¹, Peter Gerwinski², Fritz Haake², Henning Schomerus²

¹Department of Theoretical Physics, Institute of Physics, Saint-Petersburg University, Saint-Petersburg 198904, Russia
²Fachbereich Physik, Universität-Gesamthochschule Essen, D-45117 Essen, Germany

Received: 12 May 1995

Abstract. We discuss semiclassical approximations of the spectrum of the periodically kicked top, both by diagonalizing the semiclassically approximated Floquet matrix F and by employing periodic-orbit theory. In the regular case when F accounts only for a linear rotation periodic-orbit theory yields the exact spectrum. In the chaotic case the first method yields the quasienergies with an accuracy of better than 3% of the mean spacing. By working in the representation where the torsional part of the Floquet matrix is diagonal our semiclassical work is mostly an application of the asymptotics of the rotation matrix, i.e. of Wigner's so-called *d*-functions.

1. Introduction

We present a semiclassical study of periodically kicked tops. Our aim are approximations for the quasienergy spectrum valid irrespective of whether the classical limit yields regular, chaotic, or mixed dynamics.

Kicked tops [1–4] are worthy of ambitious endeavors for various reasons: (i) The finite dimension of their Hilbert space precludes the appearance of infinities in periodic-orbit expansions à la Gutzwiller. (ii) The Hilbert space dimension is a measure of (the inverse of) Planck's constant and therefore yields a convenient handle for implementing the semiclassical limit. (iii) The accuracy of semiclassical approximations is easily checked since, again due to the finite dimension of the Hilbert space, the exact quasienergy spectrum is readily obtained numerically. (iv) Under conditions of chaos the fluctuations in the quasienergy spectrum are particularly faithful to the predictions of random-matrix theory; such tops may thus said to display generic quantum chaos. (v) A good semiclassical understanding of the top might eventually give clues to a semiclassical theory of localization inasmuch as the prototypical system with quantum localization, the kicked rotator, is but a special case of the top. (vi) Another special case is linear rotation and here the unitary Floquet operator has Wigner's well-known dfunctions as matrix representatives. Interestingly, semiclassical theory gives approximate eigenfunctions but the exact Floquet spectrum in this regular case, reminding one of what

happens to the harmonic oscillator or the hydrogen atom in semiclassical treaments.

The dynamical variables of our tops are the components of an angular momentum **J** which obey the commutation relations $[J_x, J_y] = iJ_z$ etc. The squared angular momentum is thus a conserved quantity, $\mathbf{J}^2 = j(j+1)$ with j integer or half integer. The quantum number j also determines the dimension of the Hilbert space as 2j + 1. The particular top to be studied here has its stroboscopic period-to-period dynamics described by the Floquet operator [2]

$$F = e^{-i\frac{k}{2j+1}J_z^2}e^{-i\beta J_y}.$$
(1.1)

One confronts a rotation by the angle β about the y-axis followed by a torsion of strength k about the z-axis; the torsion may obviously be interpreted as a rotation by an angle proportional to J_z . Since for vanishing torsion strength, k = 0, we deal with the classically regular case of pure rotation it is the element of nonlinearity present in the generator J_z^2 of the torsion which, together with the factorization of F into a rotational and a torsional term, makes possible chaotic behavior of the classical version of the top. We would like to emphasize that with respect to earlier papers we have here changed the torsion generator by replacing the quantum number j with the semiclassical magnitude j + 1/2 of the angular momentum, writing k/(2j + 1) instead of k/2j. This slight change yields an important simplification of the semiclassical matrix elements and trace of F.

Two semiclassical paths towards the Floquet spectrum have been explored. The traditional one proceeds through semiclassical approximations for the traces of powers of the Floquet operator, tr F^n , with the integer exponent ranging from n = 1 to n = j for integer j and to $n = j + \frac{1}{2}$ for halfinteger j. This is the variant of Gutzwiller's periodic-orbit theory pertinent to periodically driven systems since the n-th such trace can be expressed semiclassically in terms of properties of period-n orbits of the classical stroboscopic dynamics. Since large values of j are required for the semiclassical approximation to become reliable one runs into the problem, in the case of classical chaos, of the exponential proliferation of periodic orbits with increasing length. Leaving the chaotic case for a future investigation we shall here employ the periodic-orbit strategy to the regular case of pure rotation. As we shall see, for generic values of the rotation angle β there is only a pair of trivial fixed points of the classical stroboscopic map which also makes up, upon *n*-fold repetition, the only period-*n* orbits and the ensuing semiclassical traces tr F^n yield the exact spectrum of the rotation matrix.

A second scheme of securing semiclassical spectra has been suggested recently [5]. It consists of approximating, in a suitable representation, all elements of the Floquet matrix which latter is then diagonalized numerically. Employing a basis formed of angular-momentum coherent states we had previously found the quasienergies for values of j ranging from about unity up to 200 in this way. The accuracy reached was surprisingly good, the typical error not exceeding 3% of the mean spacing under conditions of global chaos and even slightly better for torsion strengths sufficiently small to secure dominantly regular classical behavior.

We here take up the method of diagonalizing the semiclassically approximated Floquet matrix but work, instead of with coherent states, in the (\mathbf{J}^2, J_z) -basis. Some interesting thoughts are tied with that change of basis. Coherent states have the intuitive appeal that their "support" in the classical phase space shrinks to a point in the classical limit $j \to \infty$. Incidentally, the phase space is the sphere $\lim_{j\to\infty} \mathbf{J}^2/j^2 = 1$ and a coherent state roughly covers an area $4\pi/(2j+1)$ on that sphere. The (2j + 1) dimensional Hilbert space of the top is of course vastly overpopulated by the coherent states: Their set is as dense as the set of points on the sphere. As a consequence, the coherent states are non-orthogonal among one another. To form a complete set one must choose some grid of 2j + 1 points on the sphere and the states located on them. A matrix element between two coherent states cannot be associated, in the classical limit, with a real solution of the classical stroboscopic map unless the location of the final state happens to be the classical image of the location of the initial state; indeed, specification of both the initial and final phase space point in general amounts to an overdetermination of the classical motion. Still, the semiclassical approximation for each matrix element of F leads to a certain stationary-phase condition which is identical in appearance with the classical stroboscopic map; inasmuch as a solution of that map determines the value of the matrix element and inasmuch as that solution is overdetermined from a classical point of view, one confronts so-called ghost orbits which run through a complexified version of the classical phase space [6, 7]. Unfortunately, the number of ghost solutions of the boundary-value problem is in general infinite and, even more deplorably, at least for not too large values of j several or even many such ghosts may make sizable contributions to a given matrix element. The coherent-state based semiclassical determination of the quasienergy spectrum of the top was therefore somewhat of a tour de force and certainly more demanding of numerical means and even mathematical finesse than the straightforward diagonalization of the unapproximated Floquet matrix. Nevertheless, the success eventually reached was enjoyable since it showed that classical chaos does not preclude validity of some semiclassical approximation; a bit of consolation for the immense amount of work could be seen in the fact that for values of j as large as, say, 100 one can hardly imagine an implementation of a periodic-orbit expansion under conditions of global chaos.

We shall here rejoice in a considerable gain of efficiency brought about by employing the familiar (2j+1) eigenstates $|j,m\rangle$ of J_z for fixed eigenvalue j(j+1) of \mathbf{J}^2 as a basis set. The eigenvalue m of J_z is related to a convenient classical phase space variable, the polar angle θ defined with respect to the z-axis as $m = \sqrt{j(j+1)}\cos\theta$; we shall take $\cos\theta$ as the classical momentum and the azimuth ϕ as the canonically conjugate coordinate. The basis state $|i, m\rangle$ can thus be visualized as the circular section of the spherical phase space with the plane of constant $\cos \theta$ which leaves the azimuth ϕ free to range in $0 < \phi < 2\pi$. Clearly then, the matrix element of the Floquet operator can be associated with a solution of the classical stroboscopic map with fixed initial and final values of the momentum, the coordinate ϕ remaining unspecified; no overdetermination of the classical orbit is incurred. Upon inspection of the boundary-value problem in question we find that roughly the fraction $(\pi \sin \beta)/4$ of all matrix elements is related to a pair of real classical orbits while the remainder do not correspond to classically allowed pairs of initial and final momenta and can therefore at best be associated with complex ghost orbits; in both cases the semiclassical matrix element takes the familiar WKB form corresponding to classically allowed or classically forbidden boundary data. Since even in the latter case we did not encounter cases where more than one ghost matters we encounter closed-form expressions for all semiclassical matrix elements which are as easy to evaluate as their exact quantum partners. Upon diagonalizing the semiclassical matrix we again encounter the fine accuracy previously met with when working with coherent states, i.e. a mean error of less than 3% of the mean spacing $2\pi/(2j+1)$ of quasienergies.

Incidentally, since the torsion part of the Floquet operator (1.1) is diagonal in the (\mathbf{J}^2, J_z) -representation all the work in determining the semiclassical Floquet matrix goes into the matrix elements of the rotation operator, often called Wigner's *d*-functions $d_{m_f,m_i}^j = \langle j, m_f | e^{-i\beta J_y} | j, m_i \rangle$. Fortunately, the semiclassical *d*-functions are well known [8, 9].

2. Quantum rotation matrix and classical map

Let us consider an initial quantum state $|j, m_i\rangle$ and imagine a rotation by the angle β about the y-axis which turns our initial state into $e^{-i\beta J_y} |j, m_i\rangle$. The probability amplitude to find some "final" value m_f of J_z in the rotated state is given by the matrix element

$$d_{m_f,m_i}^j(\beta) = \langle j, m_f | e^{-i\beta J_y} | j, m_i \rangle.$$
(2.1)

A semiclassical image of the final state $|j, m_f\rangle$ is the cone of possible directions of the angular-momentum vector of length

$$\sqrt{j(j+1)} \approx j + 1/2 \equiv J \tag{2.2}$$

and projection m_f on the z-axis (see Fig. 1). This cone has the z-axis as its symmetry axis; its semiangle at the top is $\theta_f = \arccos(m_f/J)$. On the other hand, the rotated state $e^{-i\beta J_y} |j, m_i\rangle$ is depicted by a cone whose axis z' lies in the x-z-plane and includes the angle β with the z-axis; its semiangle at the top is $\theta_i = \arccos(m_i/J)$. The event whose probability amplitude equals Wigner's d-function corresponds semiclassically to the crossings of these two cones.



Fig. 1. Cones of the angular-momentum vector for the rotated initial state $\exp(-i\beta J_y)|m_i\rangle$ and reference state $|m_f\rangle$, for $\beta = \pi/2$. Their lines of intersection are the semiclassical image of the event characterized by Wigner's *d*-function; they also indicate the two final directions of the angular momentum possible for the given initial and final polar angles θ_i , θ_f . The three images belong to three different matrix elements: **a** within the classically allowed region, **b** on the elliptic border $J^2 \sin^2 \beta - m_i^2 - m_f^2 + 2m_i m_f \cos \beta = 0$ which actually is a circle in the case $\beta = \pi/2$ (see Sect. 3), and **c** in the classically forbidden region with no intersection between the cones. The symbolic equation depicts the location of the matrix elements pertaining to the cones **a**, **b**, **c**

There are two, one, or no lines of crossing if the sum of the polar angles $\theta_f + \theta_i$ is larger than, equal to, or smaller than β . If there is no crossing, the *d*-function becomes exponentially small.

We now proceed to the classical map describing the rotation of the vector **J** by the angle β about the *y*-axis. The spherical angles θ_i, ϕ_i of the initial vector are mapped into θ_f, ϕ_f as

$$\cos \theta_f = \cos \theta_i \cos \beta - \sin \theta_i \cos \phi_i \sin \beta$$

$$\sin \theta_f \cos \phi_f = \cos \theta_i \sin \beta + \sin \theta_i \cos \phi_i \cos \beta$$

$$\sin \theta_f \sin \phi_f = \sin \theta_i \sin \phi_i.$$
(2.3)

We can speak of a trajectory drawn out between the initial pair θ_i , ϕ_i and the final pair θ_f , ϕ_f as the rotation angle grows from zero to β . Suppose now that we do not fix the initial angles but instead the polar angles (θ_i , θ_f) of both the initial and final angular momentum. To identify the trajectories connecting these boundary data we must seek the azimuthal angles ϕ_i , ϕ_f . To that end we may again resort to Fig. 1; the intersection(s) of the two cones specify the final direction(s) of the angular momentum compatible with classically specified initial and final polar angles, θ_i , θ_f . The corresponding final azimuths are zero, one, or two in number and read, in the latter two cases,

$$\phi_f^{\pm} = \pm \arccos \frac{m_i - m_f \cos \beta}{\sin \beta \sqrt{J^2 - m_f^2}},\tag{2.4}$$

with $m_{i,f} = J \cos \theta_{i,f}$. The initial directions of the angular momentum can be obtained from the final ones by the inverse rotation (by the angle $-\beta$ about the y-axis, after interchanging m_i and m_f). Their azimuths are thus

$$\phi_i^{\pm} = \pm \arccos \frac{m_i \cos \beta - m_f}{\sin \beta \sqrt{J^2 - m_i^2}}.$$
(2.5)

Here and throughout the paper we assume that the inverse trigonometric functions are given by their principal values and that the azimuths are limited to the interval $[-\pi, \pi]$. Obviously, the two final points as well as the two initial points are reflections of one another in the *x*-*z*-plane.

It is worth emphasizing the important difference between the initial-value problem (θ_i, ϕ_i given) and the boundaryvalue problem (θ_i, θ_f given): while the former has a unique solution (θ_f, ϕ_f), the boundary-value problem has, in general, two different solutions (ϕ_i^+, ϕ_f^+) and (ϕ_i^-, ϕ_f^-). Of course, the continuous trajectories leading from the initial points to the final ones as the rotation angle is increased from zero to β are also two in number and run symmetrically with respect to the *x*-*z*-plane.

The classical rotation (2.3) can be looked upon as a canonical transformation for the pair of variables $m = J \cos \theta$, ϕ with the generating function

$$S_{0}(m_{f}, m_{i}) = \frac{m_{i}}{J} \arccos \frac{m_{i} \cos \beta - m_{f}}{\sin \beta \sqrt{J^{2} - m_{i}^{2}}} - \frac{m_{f}}{J} \arccos \frac{m_{i} - m_{f} \cos \beta}{\sin \beta \sqrt{J^{2} - m_{f}^{2}}} + \arccos \frac{m_{f} m_{i} - J^{2} \cos \beta}{\sqrt{(J^{2} - m_{f}^{2})(J^{2} - m_{i}^{2})}}.$$
 (2.6)

That function also has the meaning of the action of the trajectory connecting the initial and final points. The derivatives of S_0 with respect to m_i, m_f yield, as the "coordinates" canonically conjugate to the "momenta" m_f, m_i , the azimuths ϕ_i^+ and $-\phi_f^+$,

$$J\partial S_0/\partial m_i = \arccos \frac{m_i \cos \beta - m_f}{\sin \beta \sqrt{J^2 - m_i^2}} = \phi_i^+$$

$$J\partial S_0/\partial m_f = -\arccos \frac{m_i - m_f \cos \beta}{\sin \beta \sqrt{J^2 - m_f^2}} = -\phi_f^+.$$
(2.7)

Replacing S_0 by $-S_0$ we obtain the other trajectory connecting the initial and final momenta, the azimuths of which are $\phi_i^- = -\phi_i^+, \ \phi_f^- = -\phi_f^+$. We shall in the following account for the two trajectories by introducing a factor $\sigma = \pm 1$ and writing σS_0 for the action.

3. WKB approximation for rotation matrix elements

In the limit of large total angular momentum, $j \gg 1$, Wigner's *d*-functions can be approximated semiclassically. Deferring a sketch of the derivation of the well-known WKB form [8, 10, 11] to Appendix A we here simply quote the result obtained for rotation angles β in the interval $[0, \pi]$,

$$d_{m_f,m_i}^j(\beta) = (-1)^j \sqrt{\frac{2J}{\pi} \left| \frac{\partial^2 S_0}{\partial m_i \partial m_f} \right|} \cos(JS_0 - \pi/4), \quad (3.1)$$

where S_0 is the classical action given in (2.6) and, again, $J = j + \frac{1}{2}$. Curiously, the connection of this well-known asymptotic form of the *d*-function with the classical rotation map (i.e. the appearance of the generating function of the classical map in the semiclassical phase of d_{m_f,m_i}^j) seems not to have been paid much attention before (see, however, Ref. [12]).

The prefactor of the cosine in the semiclassical d-function (3.1) involves the second mixed derivative

$$\frac{\partial^2 S_0}{\partial m_i \partial m_f} = \frac{1}{J} \frac{\partial \phi_i}{\partial m_f}$$
$$= \frac{1}{J\sqrt{J^2 \sin^2 \beta - m_i^2 - m_f^2 + 2m_i m_f \cos \beta}}.$$
(3.2)



Fig. 2. Elliptic boundary of classically allowed transitions in the m_i - m_f -plane. The gray shade indicates, for j = 50 and $\beta = 1$, the squared modulus of the matrix element: One sees rapid oscillations inside the classically allowed region and exponential decay outside

The semiclassical approximation (3.1) is valid when the transition $m_i \rightarrow m_f$ is classically allowed, i. e. when the cones in Fig. 1 intersect. According to the geometrical interpretation given above the classically accessible range of the quantum numbers m_f , m_i can be characterized by the inequality $\theta_f + \theta_i \ge \beta$ which implies

$$R(m_f, m_i) \equiv J^2 \sin^2 \beta - m_i^2 - m_f^2 + 2m_i m_f \cos \beta > 0.$$
(3.3)

This inequality determines the area inside an ellipse in the $m_i \cdot m_f$ -plane inscribed into the square $-J \leq m_i, m_f \leq J$. It is easy to see that the axes of the ellipse coincide with the diagonals of the square and that its semiaxes are $\sqrt{2}J\cos(\beta/2)$ and $\sqrt{2}J\sin(\beta/2)$. The ellipse touches the boundary of the square in the four points $(m_i, m_f) = (\pm J, \pm J\cos\beta), (\pm J\cos\beta, \pm J)$. In the special case of a rotation by $\beta = \pi/2$ the ellipse turns into a circle. Each integer point (m_i, m_f) within the elliptic region (3.3) corresponds to a pair of classical trajectories. The points outside of the region (3.3) determine trajectories with complex initial and final azimuths and are consequently of the "ghost" type [6, 7]. Forbidden pairs have complex actions S_0 and thus exponentially small values of the d-function.

At the boundary of the classically allowed domain, $R(m_f, m_i) = 0$, the second mixed derivative of the action S_0 (3.2) and thus the naive WKB approximation (3.1) diverge. This well-known breakdown is overcome by the so-called *uniform* WKB approximation [13] the derivation of which we also briefly comment on in Appendix A. It suffices to write down the uniformly approximated *d*-function under the restriction

$$0 < \beta < \pi/2, \quad m_i > 0, \quad |m_f| < m_i,$$
 (3.4)

since the symmetry properties

$$d_{m_f,m_i}^{j}(\beta) = (-1)^{m_f - m_i} d_{m_i,m_f}^{j}(\beta)$$

= $d_{-m_i,-m_f}^{j}(\beta) = (-1)^{m_f - m_i} d_{m_f,m_i}^{j}(-\beta)$
= $(-1)^{j - m_i} d_{-m_f,m_i}^{j}(\pi - \beta)$ (3.5)

yield the *d*-functions outside these limitations. The uniformly approximated matrix element then takes two slightly different forms depending on the sign of $m_f - m_i \cos \beta$. First consider

$$m_f < m_i \cos \beta. \tag{3.6}$$

Then the Airy function Ai (λ) appears as

$$d_{m_f m_i}^j(\beta) = \left[\frac{-4\lambda}{R(m_f, m_i)}\right]^{1/4} \operatorname{Ai}(\lambda).$$
(3.7)

For classically allowed index pairs $(R(m_f, m_i) > 0)$ the argument λ of the Airy function is expressed in terms of the classical action as

$$\lambda = -\left\{\frac{3}{2}J\left[\pi - S_0(m_f, m_i)\right]\right\}^{2/3},$$
(3.8)

while in the classically forbidden region $\pi - S_0$ is imaginary and we have

$$\lambda = \left\{\frac{3}{2}J\mathrm{Im}\left[-S_0(m_f, m_i)\right]\right\}^{2/3}$$
(3.9)

with

$$\operatorname{Im}\left[-S_{0}(m_{f}, m_{i})\right] = -\frac{m_{f}}{J}\operatorname{arcosh}\frac{m_{i} - m_{f}\cos\beta}{\sin\beta\sqrt{J^{2} - m_{f}^{2}}}$$
$$+\frac{m_{i}}{J}\operatorname{arcosh}\frac{|m_{i}\cos\beta - m_{f}|}{\sin\beta\sqrt{J^{2} - m_{i}^{2}}}$$
$$-\operatorname{arcosh}\frac{|m_{f}m_{i} - J^{2}\cos\beta|}{\sqrt{(J^{2} - m_{f}^{2})(J^{2} - m_{i}^{2})}}.$$
(3.10)

Recalling that we have just specified the uniform WKB approximation assuming $m_f < m_i \cos \beta$, we now turn to the opposite case, $m_f \ge m_i \cos \beta$. The following modifications must be made in the expressions given: (i) The factor $(-1)^{j-m_i}$ should be introduced in the r.h.s. of (3.7); (ii) in (3.8) $\pi - S_0$ should be replaced by $S_0 - (m_i/J)\pi$; (iii) the sign of the first term in the r.h.s. of (3.10) should be changed.

It is worth noting that, for m_f , m_i considered continuous, the two definitions (3.8,3.9) of the argument λ of the Airy function join smoothly at the elliptic border $R(m_f, m_i) = 0$ of the classically allowed and forbidden regions in the m_f m_i -plane. In fact, λ vanishes identically on that line; this is most easily seen when approaching the border from the classically forbidden region; according to $R(m_f, m_i) = 0$, the arguments of all three inverse hyperbolic functions in (3.10) are equal to unity such that indeed Im $S_0 = 0$ and thus $\lambda = 0$ on the elliptic border line. Reasoning similarly when approaching the ellipse from within its classically allowed inside, one finds $S_0 = \pi$ and thus again $\lambda = 0$.

It is well known that the WKB approximation loses its accuracy for the wave function of the ground state of an autonomous quantum system, due to the close approach of two turning points of the classical motion. For the same reason, semiclassical approximations for Wigner's *d*-functions (including the uniform approximation (3.7)) become inaccurate when a pair (m_f, m_i) approaches any one of the four points of tangency between the ellipse limiting the classically allowed region and the lines $m_f, m_i = \pm J$. Near these points improved asymptotics can be obtained through the so-called harmonic-oscillator approximation [9]. As we indicate in Appendix A, the *d*-function with m_i fixed then obeys a second-order differential equation with the independent variable m_f . That differential equation turns out as the Schrödinger equation for the harmonic oscillator with $\hbar = 1$, mass $m = (J \sin^2 \beta)^{-1}$, and frequency $\omega = 1$. Denoting its eigenfunctions by $\psi_n(x)$ we obtain, near the tangency point $m_i = J \approx j$, $m_f = J \cos \beta$,

$$d_{m_f,m_i}^j(\beta) \approx \psi_{j-m_i}(J\cos\beta - m_f). \tag{3.11}$$

The behavior near the other three points of tangency can be obtained through the symmetry relations (3.5).

4. Semiclassical trace of the Floquet operator

At this point we generalize our discussion to the kicked top with the Floquet operator (1.1). Of course, the case of pure linear rotation is recovered by setting the torsion strength kequal to zero. We are interested in the semiclassical limit of the spectrum of the Floquet operator F which can be obtained if we know the characteristic polynomial of F. Coefficients of the latter are simply connected with the traces of the powers of the operator F, i. e. tr F, tr F^2 , ..., tr F^j [14]. We shall show that tr F^n can be expressed through the actions of the period-n solutions of the map corresponding to the operator F in the classical limit. This map describes a rotation about the y-axis by β (see (2.5)) followed by a nonlinear torsion about the z-axis. The latter leads to an increment of the azimuth ϕ_f proportional to m_f so that the composite transformation reads

$$\theta_{i} = \arccos(m_{i}/J), \quad \phi_{i}^{\pm} = \pm \arccos\frac{m_{i}\cos\beta - m_{f}}{\sin\beta\sqrt{J^{2} - m_{i}^{2}}}$$
$$\theta_{f} = \arccos(m_{f}/J),$$
$$\phi_{f}^{\pm} = \pm \arccos\frac{m_{i} - m_{f}\cos\beta}{\sin\beta\sqrt{J^{2} - m_{f}^{2}}} + (k/J)m_{f}. \tag{4.1}$$

The angle ϕ_f in the equations (2.3) should likewise be increased by $(k/J)m_f$.

Let us begin by calculating the semiclassical value of the trace of the first power of F. With the help of the $|jm\rangle$ -basis we may write

tr
$$F = \sum_{m} e^{-ikm^2/(2J)} d^j_{m,m}(\beta).$$
 (4.2)

We here replace the Wigner functions by their WKB asymptotics and thus obtain a sum of terms which may be considered as continuous functions of the quantum number m. We then invoke Poisson's formula to replace the summation over m by a sum of integrals over m,

$$\sum_{m=-j}^{j} f(m) = \sum_{n=-\infty}^{\infty} \int_{-j-1/2}^{j+1/2} dm f(m) e^{-i2\pi nm}.$$
 (4.3)

We shall use the simple semiclassical asymptotics (3.1) for the *d*-functions. Employing, instead of *m*, the "classical" integration variable $\xi = m/J$, we introduce the total classical action $S(\xi_f, \xi_i, \sigma)$ which includes the rotational part S_0 defined in the previous section and the torsional part $k\xi_f^2/2$,

$$S(\xi_f, \xi_i, \sigma) = \sigma S_0(J\xi_f, J\xi_i) - \frac{k\xi_f^2}{2} =$$

$$= \sigma \left[\xi_i \arccos \frac{\xi_i \cos \beta - \xi_f}{\sin \beta \sqrt{1 - \xi_i^2}} - \xi_f \arccos \frac{\xi_i - \xi_f \cos \beta}{\sin \beta \sqrt{1 - \xi_f^2}} \right]$$

$$+ \arccos \frac{\xi_f \xi_i - \cos \beta}{\sqrt{(1 - \xi_f^2)(1 - \xi_i^2)}} - \frac{k\xi_f^2}{2}. \quad (4.4)$$

We recall that the discrete variable $\sigma = \pm 1$ serves to distinguish the two symmetric classical trajectories arising for fixed initial and final polar angles. Obviously, the torsional part of the action yields the correct shift $km_f/J = k\xi_f$ of the final azimuth through $\phi_f = -\partial S/\partial\xi_f$. Our trace (4.2) now takes the semiclassical form

$$\operatorname{tr} F = (-1)^{j} \sum_{\sigma = \pm 1} \sum_{n} \int d\xi$$
$$\times \sqrt{\frac{J}{2\pi} \left| \frac{\partial^{2} S}{\partial \xi_{f} \partial \xi_{i}} \right|_{\xi_{f} = \xi_{i} = \xi}} e^{i J[S(\xi, \xi, \sigma) - 2\pi n\xi] - i\sigma \pi/4}.$$
(4.5)

Since the second mixed derivative of the torsional part of S vanishes identically we could express the normalizing factor of the d-function in terms of S rather than the rotational action S_0 . Thus, the derivative in the radicand of (4.5) has the explicit form

$$\frac{\partial^2 S(\xi_f, \xi_i, \sigma)}{\partial \xi_f \partial \xi_i} \bigg|_{\xi_f = \xi_i = \xi} = \frac{\sigma}{\sqrt{\sin^2 \beta - 2\xi^2 (1 - \cos \beta)}}.$$
 (4.6)

To fully implement the semiclassical approximation we treat each integral in the sum (4.5) by the stationary-phase method. The points of stationary phase are determined by $(d/d\xi)[S(\xi,\xi,\sigma) - 2\pi\xi n] = 0$ or, more explicitly, by

$$\frac{k\xi}{2} + \pi n = \sigma \arcsin \frac{\xi(1 - \cos\beta)}{\sin\beta\sqrt{1 - \xi^2}}.$$
(4.7)

A solution of that equation (4.7) yields a fixed point of the classical map (4.1). In fact, calculating the trace we set $m_i = m_f = m$ which means equality of the initial and final polar angles. On the other hand, from

$$\frac{d}{d\xi} \left[S(\xi,\xi,\sigma) - 2\pi n\xi \right]$$

= $\sigma \left[\phi_i^{\sigma}(m,m) - \phi_f^{\sigma}(m,m) \right]_{m=J\xi} - 2\pi n$
= $\left[\phi_i^{\sigma}(m,m) - \phi_f^{\sigma}(m,m) \right]_{m=J\xi} - 2\pi n$ (4.8)

we see that the stationary-phase condition (4.7) implies equality modulo 2π of the initial and final azimuths.

To determine a fixed point θ_a , ϕ_a from (4.7) for given values of k, β , σ it is convenient to take the tangent of both sides of that equation, thus eliminating the multiple of π . Of course, $\sigma = \sigma_a$ equals the sign of ϕ_a . Once a fixed point θ_a , ϕ_a is found one may return to the stationary-phase equation in the original form (4.7) and determine the integer $n = n_a$ from our convention for the inverse trigonometric functions, i.e. such that $k\xi/2 + \pi n_{\alpha}$ lies in the interval $[-\pi/2, \pi/2]$. It is with that and only that value n_a of n that the fixed point in question makes a non-negligible contribution to the sum over n in the semiclassical trace (4.5). We are now all set to employ the stationary-phase approximation for the integrals in the trace (4.5). For smooth functions $f(\xi)$ and $g(\xi)$ and with ξ_a denoting the roots of $f'(\xi_a) = 0$, $a = 0, 1, 2, \ldots$, the asymptotic approximation in question yields, in the limit of large J,

$$\int d\xi g(\xi) e^{iJf(\xi)} \approx \sum_{a} \sqrt{\frac{2\pi}{J|f''(\xi_a)|}} g(\xi_a) e^{iJf(\xi_a) \pm i\pi/4},$$
(4.9)

where the sign before $i\pi/4$ should be the same as that of $f''(\xi_a)$. Applying this to the trace (4.5) we obtain the Gutzwiller type result

$$\operatorname{tr} F' = (-1)^{j} \sum_{a} \\ \times \sqrt{\left| \frac{1}{S_{a}''} \frac{\partial^{2} S}{\partial \xi_{f} \partial \xi_{i}} \right|_{\xi_{f} = \xi_{i} = \xi_{a}}} e^{i [J(S_{a} - 2\pi n_{a}\xi_{a}) - \alpha_{a}\pi/2]}.$$
(4.10)

Here we denote by S_a the value of the action $S(\xi, \xi, \sigma)$ and by S_a'' the value of the second total derivative $d^2S(\xi, \xi, \sigma)/d\xi^2$ at the point ξ_a, σ_a . The integer Maslov index α_a can take on the values $0, \pm 1$ and reads $\alpha_a = (\sigma_a - \mu_a)/2$ with $\mu_a = \pm 1$ the sign of S_a'' [15]. The sum is taken over all fixed points of the map.

The radicand in (4.10) can be expressed in terms of the trace of the so-called monodromy matrix,

$$\operatorname{tr} M = \left(\frac{\partial \phi_f}{\partial \phi_i}\right)_{\xi_i} + \left(\frac{\partial \xi_f}{\partial \xi_i}\right)_{\phi_i}.$$
(4.11)

To that end we once more employ the action in its role as a generating function, $\partial S/\partial \xi_i = \phi_i$, $\partial S/\partial \xi_f = -\phi_f$, and infer, with a bit of calculus, the desired identity

$$\frac{1}{S_a''} \frac{\partial^2 S(\xi_f, \xi_i, \sigma)}{\partial \xi_f \partial \xi_i} \bigg|_{\xi_f = \xi_i = \xi}$$
$$= \left[2 + \frac{\left(\frac{\partial \phi_i}{\partial \xi_i}\right)_{\xi_f} - \left(\frac{\partial \phi_f}{\partial \xi_f}\right)_{\xi_i}}{\left(\frac{\partial \phi_i}{\partial \xi_f}\right)_{\xi_i}} \right]^{-1} = (2 - \operatorname{tr} M)^{-1}. \quad (4.12)$$

Substituting the expression for S_a and again invoking the stationary-phase condition (4.7), we arrive at the fully explicit form of our semiclassical trace,

$$\operatorname{tr} F = (-1)^{j} \\ \times \sum_{a} \left| \frac{2(1 - \cos \beta)}{1 - \xi_{a}^{2}} - \sigma_{a} k \sqrt{\sin^{2} \beta - 2\xi_{a}^{2}(1 - \cos \beta)} \right|^{-1/2} \\ \times \exp \left[i J \left(k \xi_{a}^{2} / 2 + \sigma \arccos \frac{\xi_{a}^{2} - \cos \beta}{1 - \xi_{a}^{2}} \right) \right.$$

$$+ i(\mu_{a} - \sigma_{a}) \pi / 4 \right].$$

$$(4.13)$$

According to (4.6), the index $\mu_a = \pm 1$ is equal to σ_a , times the sign of 2 - tr M (the expression in the modulus brackets). The reader should wonder about the disappearance of the phase $-2\pi n_a \xi_a$ on the way from (4.10) to (4.13) but will check easily that when invoking the stationary-phase



Fig. 3. Real part of the exact and the semiclassical trace and modulus of the error, $|(tr F)_{S,C} - tr F|$, versus the torsion constant k for $\beta = \pi/2$, j = 250. The error is negligible except for the neighborhoods of the bifurcations at k = 2 and k = 12.73

equation (4.7) we had to stick to our convention that all inverse trigonometric functions are meant with their principal values.

In general, fixed points of the map have to be found by numerically solving (4.7). Exceptions are represented by the two trivial points $\theta = \pi/2$, $\phi = \pm \pi/2$, or $\xi = 0, \sigma = \pm 1$, which exist regardless of k. If $k < 2 \tan \frac{\beta}{2}$, these are the only fixed points, and the Gutzwiller development (4.13) acquires a particularly simple form,

$$\operatorname{tr} F \approx \frac{1}{i} \left[\frac{e^{iJ\beta}}{\sqrt{2(1 - \cos\beta) + k\sin\beta}} - \frac{e^{-iJ\beta}}{\sqrt{2(1 - \cos\beta) - k\sin\beta}} \right].$$
(4.14)

In the case of pure rotation (k = 0) this formula gives the exact value of the trace of the rotation matrix. We shall come back to that special case in a separate section below.

As an example we have evaluated tr *F* for the case $\beta = \pi/2$, j = 250 as a function of the torsion constant *k*. As Fig. 3 shows, the results provided by the Gutzwiller development (4.13) and by the "exact" numerical calculation agree well, except in the vicinity of the zeros of tr M(k) - 2 where the semiclassical expression diverges. Such zeros correspond to classical bifurcations at which new fixed points are born.

It is interesting to follow, in Fig. 3, the behavior of the trace tr F(k) through the sequence of bifurcations. In the range 0 < k < 2 there exist only the two trivial periodic points already mentioned; the trace, given by (4.14), then

varies with k only via the prefactor, i.e. slowly and monotonically. In the subsequent range 2 < k < 12.73, two new fixed points (which differ only in the sign of ξ) contribute a single oscillating summand in (4.13). With the advent of further fixed points at k = 12.73 more oscillating terms arise whereupon the k dependence of tr F becomes more erratic.

5. Two-step propagator

In order to prepare for the semiclassical evaluation of traces of arbitrary powers of the Floquet operator F we here consider the trace of F^2 which is connected to the once iterated classical map. The matrix element of F^2 is given by

$$\langle m_3 | F^2 | m_1 \rangle = \sum_{m_2} d^j_{m_3, m_2} d^j_{m_2, m_1} e^{-ik(m_3^2 + m_2^2)/2J} .$$
 (5.1)

We now proceed in analogy to the foregoing treatment of tr F: First, we employ the semiclassical versions (3.1,2.6) of the Wigner functions $d_{m,m'}^j$. With the help of Poisson's identity we then convert the sum over m_2 into an integral over a continuous variable and introduce the rescaled quantities $\xi_i = m_i/J$, thus obtaining

$$\langle m_3 | F^2 | m_1 \rangle = \sum_{n_2} \sum_{\{\sigma_i = \pm 1\}} (2\pi)^{-1} \int d\xi_2$$
$$\times \sqrt{\left| \frac{\partial^2 S(\xi_3, \xi_2, \sigma_2)}{\partial \xi_3 \partial \xi_2} \frac{\partial^2 S(\xi_2, \xi_1, \sigma_1)}{\partial \xi_2 \partial \xi_1} \right|}$$

$$\times \exp\left\{ iJ\left(S(\xi_3,\xi_2;\sigma_2) + S(\xi_2,\xi_1;\sigma_1) - 2\pi n_2\xi_2\right) - i\frac{\pi}{4}(\sigma_1 + \sigma_2) \right\}.$$
(5.2)

We shall eventually evaluate the ξ_2 integral in the stationaryphase approximation. As a preparation to this step and similar ones to be taken later we adopt the notation $S_2(\xi_3, \xi_2) \equiv$ $S(\xi_3, \xi_2; \sigma_2)$ and $S_1(\xi_2, \xi_1) \equiv S(\xi_2, \xi_1; \sigma_1)$ and do not even assume, momentarily, any special form of S_1 and S_2 . Stationary-phase values of ξ_2 are determined by

$$\frac{\partial S_2(\xi_3,\xi_2)}{\partial \xi_2} + \frac{\partial S_1(\xi_2,\xi_1)}{\partial \xi_2} - 2\pi n_2 = 0.$$
 (5.3)

This implies that the initial point of the transformation generated by S_2 is the final point of the transformation generated by S_1 ; indeed, the two polar angles θ_i, θ_f in question are both equal to $\arccos \xi_2$ while the foregoing stationary-phase condition equates the two azimuths ϕ_i, ϕ_f , up to an integer multiple of 2π .

Through a reasoning similar to the one given in the previous section the stationary-phase equation yields $\xi_2 = \xi_2(\xi_3, \xi_1)$ and the integer n_2 as functions of ξ_3 and ξ_1 . (There may be several solutions ξ_2 , n_2 .) With this in mind we can bring the matrix element of F^2 into a form analogous to the one of F itself. To proceed towards this goal, we differentiate (5.3) with respect to ξ_3 and multiply by $\partial \xi_2/\partial \xi_1$, thus obtaining

$$\frac{\partial \xi_2}{\partial \xi_1} \frac{\partial \xi_2}{\partial \xi_3} \left(\frac{\partial^2 S_2(\xi_3, \xi_2)}{\partial \xi_2^2} + \frac{\partial^2 S_1(\xi_2, \xi_1)}{\partial \xi_2^2} \right) = -\frac{\partial^2 S_2(\xi_3, \xi_2)}{\partial \xi_2 \partial \xi_3} \frac{\partial \xi_2}{\partial \xi_1} \equiv A .$$
(5.4)

In the same manner, by taking the derivative with respect to ξ_1 and multiplying with $\partial \xi_2 / \partial \xi_3$ we get $A = (-\partial^2 S_1(\xi_2, \xi_1) / \partial \xi_2 \partial \xi_1) (\partial \xi_2 / \partial \xi_3)$. A third equation for the auxiliary quantity A is obtained with the help of the action of the composite map,

$$S^{(2)}(\xi_3,\xi_1) = S_2(\xi_3,\xi_2(\xi_3,\xi_1)) + S_1(\xi_2(\xi_3,\xi_1),\xi_1) - 2\pi n_2 \xi_2(\xi_3,\xi_1) , \qquad (5.5)$$

by taking the mixed second derivative to yield $A = -(\partial^2 S^{(2)}(\xi_3, \xi_1)/\partial \xi_3 \partial \xi_1).$

The stationary-phase approximation to the ξ_2 integral in the matrix element (5.2) brings the second derivative with respect to ξ_2 of the phase $S_2(\xi_3, \xi_2) + S_1(\xi_2, \xi_1)$ into the square-root factor in front of the exponential; the sign of this derivative will later be denoted by $\mu_{3,1}$. The resulting combined radicand can be transformed using the three foregoing identities for the auxiliary quantity A to yield

$$\frac{\frac{\partial^2 S_2(\xi_3,\xi_2)}{\partial \xi_3 \partial \xi_2} \frac{\partial^2 S_1(\xi_2,\xi_1)}{\partial \xi_2 \partial \xi_1}}{\frac{\partial^2 S_2(\xi_3,\xi_2)}{\partial \xi_2^2} + \frac{\partial^2 S_1(\xi_2,\xi_1)}{\partial \xi_2^2}} = -\frac{\partial^2 S^{(2)}(\xi_3,\xi_1)}{\partial \xi_3 \partial \xi_1} .$$
(5.6)

We thus arrive at the semiclassical matrix element of F^2 ,

$$\langle m_3 | F^2 | m_1 \rangle = \sum_{\sigma_1, \sigma_2} (2\pi J)^{-1/2} \sum_{\substack{\text{saddle} \\ \text{points}}} \left| \frac{\partial^2 S^{(2)}(\xi_3, \xi_1)}{\partial \xi_3 \partial \xi_1} \right|^{1/2}$$

$$\times \exp\left\{iJS^{(2)}(\xi_3,\xi_1) + i\frac{\pi}{4}(-\sigma_1 - \sigma_2 + \mu_{3,1})\right\}.$$
 (5.7)

This semiclassical expression for the composite map resembles the WKB formula (3.1) for the simple matrix element $\langle m_2 | F | m_1 \rangle$.

For the calculation of the trace $\sum_{m} \langle m | F^2 | m \rangle$ we once more invoke Poisson's identity and the stationary-phase approximation. In analogy to the first trace we encounter an amplitude factor $|2 - \operatorname{tr} M^{(2)}|^{-1/2}$ involving the trace

$$\operatorname{tr} M^{(2)} = \left(\frac{\partial \phi_3}{\partial \phi_1}\right)_{m_1} + \left(\frac{\partial m_3}{\partial m_1}\right)_{\phi_1}$$
(5.8)

of the monodromy matrix $M^{(2)}$ of the once iterated map. The final result takes the form of a sum over all periodic points of period 2 of the classical map,

tr
$$F^2 = \sum_{\text{points}} \left| 2 - \text{tr} M^{(2)} \right|^{-1/2} \exp\left\{ i J S^{(2)} - i \alpha \frac{\pi}{2} \right\}.$$
 (5.9)

Here α denotes the integer Maslov index of the fixed point of the iterated map, $\alpha = (\sigma_1 + \sigma_2 - \mu_{1,3} - \mu^{(2)})/2$, and $\mu^{(2)} = \pm 1$ is the sign of the second total derivative of the action $S^{(2)}(\xi_1, \xi_1)$ of the composite map with equal arguments. The sum is to be taken over all periodic points of period 2, each of which is an orbit $\theta_1, \phi_1 \rightarrow \theta_2, \phi_2 \rightarrow \theta_1, \phi_1$, with σ_1, σ_2 equal to the signs of the azimuths ϕ_1, ϕ_2 . Of course, fixed points are to be included as special cases of period-2 points as well.

With the help of the intervening stationary-phase equations we simplify the action $S^{(2)}$ of the composite map as

$$S^{(2)}(\xi_3,\xi_1;\{\sigma_1,\sigma_2\})\big|_{\xi_3=\xi_1} = (\sigma_1+\sigma_2)\arccos\frac{\xi_1\xi_2-\cos\beta}{\sqrt{(1-\xi_1^2)(1-\xi_2^2)}} + \frac{k}{2}(\xi_1^2+\xi_2^2).$$
 (5.10)

Just like for the matrix element, we meet with a semiclassical expression for tr F^2 resembling the one obtained in the previous section for tr F. We are now prepared to establish semiclassical approximations of this type for the matrix elements and the trace of the multiply iterated map F^n .

6. Traces of higher powers of the Floquet operator

Since in the discussion of the stationary-phase condition (5.3) we did not specify the actions S_1 and S_2 , we can simply adapt these considerations to the traces of higher powers of the F. We start from the matrix element

$$\langle m_{n+1} | F^n | m_1 \rangle = \sum_{\{m_2...m_n\}} \prod_{j=1}^n d^j_{m_{j+1},m_j} e^{-ikm^2_{j+1}/2J}$$
. (6.1)

In the same spirit as above we express the Wigner functions by their WKB asymptotics for large J and use Poisson's identity to transform sums into integrals. After introducing the scaled variables $\xi_i = m_i/J$ the integrations can be performed step by step using the stationary-phase approximation. At the *i*-th integration we incur the action $S^{(i)}$ of the i-1 times iterated map which is related to the action $S^{(i-1)}$ by

$$S^{(i)}(\xi_{i+1},\xi_1) = S_i(\xi_{i+1},\xi_i(\xi_{i+1},\xi_1)) + S^{(i-1)}(\xi_i(\xi_{i+1},\xi_1),\xi_1) - 2\pi n_i \xi_i(\xi_{i+1},\xi_1).$$
(6.2)

Moreover, each semiclassical integration brings in a Maslov index $\mu_{i+1,1} = \pm 1$, determined by the sign of the second partial derivative with respect to ξ_i of the sum $S_i(\xi_{i+1}, \xi_i) + S^{(i-1)}(\xi_i, \xi_1)$.

Having performed all integrations in the matrix element (6.1) we arrive at its semiclassical version

$$\langle m_{1} | F^{n} | m_{n+1} \rangle$$

$$= (-1)^{jn} \sum_{\{\sigma_{i}=\pm 1\}} \exp\left(-i\frac{\pi}{4}\sum_{i=1}^{n}\sigma_{i}\right) \left(\frac{J}{2\pi}\right)^{1/2}$$

$$\times \sqrt{\left|\frac{\partial^{2}S^{(n)}(\xi_{n+1},\xi_{1})}{\partial\xi_{1}\partial\xi_{n+1}}\right|}$$

$$\times \exp\left\{iJS^{(n)}(\xi_{n+1},\xi_{1}) + i\frac{\pi}{4}\sum_{i=2}^{n}\mu_{i+1,1}\right\}.$$

$$(6.3)$$

Here $S^{(n)}$ denotes the action of the n-1 times iterated classical map,

$$S^{(n)}(\xi_{n+1},\xi_1) = \sum_{i=1}^n S(\xi_{i+1}(\xi_{n+1},\xi_1),\xi_i(\xi_{n+1},\xi_1);\sigma_i) -2\pi \sum_{i=2}^n n_i \xi_i(\xi_{n+1},\xi_1), \qquad (6.4)$$

where all intermediate ξ_i are determined as functions of ξ_1 and ξ_{n+1} by successively using the stationary-phase equation. Obviously, the matrix element maintains its WKB form previously established for n = 1, 2; the same must hold true for the trace $\sum_m \langle m | F^n | m \rangle$, which thus takes the form

$$\operatorname{tr} F^{n} = (-1)^{jn} \sum_{\text{points}} |2 - \operatorname{tr} M^{(n)}|^{-1/2} \\ \times \exp\left\{ i J S^{(n)} - i \frac{\pi}{2} \alpha \right\} .$$
(6.5)

Here we have to sum over all periodic points of period n with $\xi_1 = \xi_{n+1}$ as they are determined by the stationaryphase equations. The points in question include those on orbits with primitive period n as well as those on sequences of orbits whose periods add up to n. The action $S^{(n)}$ is a simple generalization of $S^{(2)}$ given in (5.10),

$$S^{(n)} = \sum_{i=1}^{n} \sigma_i \arccos \frac{\xi_i \xi_{i+1} - \cos \beta}{\sqrt{(1 - \xi_i^2)(1 - \xi_{i+1}^2)}} + \frac{k}{2} \sum_{i=1}^{n} \xi_i^2 . \quad (6.6)$$

The integer Maslov index of a period-*n* point reads $\alpha = \frac{1}{2} \left(\sum_{i=1}^{n} \sigma_i - \sum_{i=2}^{n} \mu_{i+1,1} - \mu^{(n)} \right)$ where $\mu^{(n)} = \pm 1$ is the sign of the second total derivative of the total action $d^2 S^{(n)}(\xi_1, \xi_1)/d\xi_1^2$ calculated at the point in consideration. The index σ_i (i = 1, ..., n) indicates the sign of the azimuth of the *i*-th intermediate point whose polar angle is $\theta_i = \arccos \xi_i$. The prefactor now contains the trace

$$\operatorname{tr} M^{(n)} = \left(\frac{\partial \phi_{n+1}}{\partial \phi_1}\right)_{m_1} + \left(\frac{\partial m_{n+1}}{\partial m_1}\right)_{\phi_1}$$
(6.7)

of the monodromy matrix $M^{(n)}$ of the n-1 times iterated map. It can be shown that the trace formula (6.5) is representation independent. In particular, following the strategy of [14] it can also be derived in the coherent-state basis [16].

7. Semiclassical spectrum of pure rotation

We now return to the case of the pure rotation, i.e. k = 0, for which both the exact form and the semiclassical approximation of tr F^n can be evaluated analytically. The exact quantum-mechanical result reads

tr
$$F^n(\beta) = \sum_{m=-j}^{j} e^{-imn\beta} = \frac{\sin n(j+1/2)\beta}{\sin n\beta/2} = \text{tr } F(n\beta).$$
 (7.1)

Much to our surprise we found the semiclassical approximation (6.5) to completely recover this exact result. Loosely speaking we may say that the semiclassical errors incurred in the matrix elements and the trace operation cancel one another in the traces. This also entails full agreement of the semiclassical spectrum of the Floquet operator with the exact one. To appreciate this somewhat peculiar situation it is well to realize a close analogy to other classically regular dynamics like the Hydrogen atom and the harmonic oscillator: There as well, the WKB approximation yields the right spectrum but fails to give the correct wave functions.

For a generic rotation, i.e. for any value of β which is not a rational multiple of 2π there are two classical fixed points, each with $\xi_i = \xi_f = 0$. These correspond to the intersection of the sphere of constant \mathbf{J}^2 and the *y*-axis and thus have $\sigma = \pm 1$. All longer periodic orbits are composed of these trivial ones. As a first step towards establishing the equality of the semiclassical and quantum traces we have checked that the identity tr $F^n(\beta) = \text{tr } F(n\beta)$ is not fouled up semiclassically. We shall not bother to write out the corresponding technical game which mostly amounts to struggling with the Maslov indices. Suffice it to say that we must start from a slightly generalized version of the semiclassical trace (4.13) which no longer requires the rotation angle to lie in the interval $[0, \pi]$,

$$\left(\operatorname{tr} F(n\beta)\right)_{\text{s.c.}} = (-1)^{j} \sum_{\text{points}} |2 - \operatorname{tr} M|^{-1/2}$$
$$\times \exp\left\{iJ\operatorname{sgn}\left(n\sin\beta\right)\sigma\right.$$
$$\times \arccos\frac{\xi^{2} - \cos n\beta}{1 - \xi^{2}} + i(\mu - \operatorname{sgn}\left(\sin n\beta\right)\sigma)\right\}.$$
(7.2)

Obviously, the factors sgn(sin $n\beta$) are the prize to pay for removing all restrictions on $n\beta$. The prefactor involving the monodromy matrix can be calculated from the classical map as

$$|2 - \operatorname{tr} M^{(1)}(n\beta)|^{-1/2} = \frac{1}{2|\sin n\beta/2|} .$$
(7.3)

Finally, the Maslov index arises within the final stationaryphase approximation as

$$\mu = \sigma \operatorname{sgn}\left(\frac{d^2 S_0(\xi,\xi)}{d\xi^2}\right) = \sigma \operatorname{sgn}(\sin n\beta).$$
(7.4)

With these ingredients one easily checks the semiclassical traces to equal the exact quantum-mechanical ones (7.1).

Lesser fortune is incurred when $n\beta$ is a multiple of 2π which means $F^n = 1$ and $d_{m,m'} = \delta_{m,m'}$. In this case the trace formula (7.1) has to be regularized to yield the value 2J. Alas, the naive WKB approximation leads to a divergent d-function since the border between the classical allowed and forbidden region degenerates to the diagonal of the matrix in this case. It is thus only for generic angles of rotation that the naive WKB approximation gives the exact Floquet spectrum.

8. Semiclassical spectrum of the kicked top

The Floquet spectrum of the periodically kicked top was recently calculated by diagonalizing the semiclassically approximated Floquet matrix, in a matrix representation based on coherent states [5]. The semiclassical limit for all matrix elements was implemented as a stationary-phase approximation in a suitable integral representation for the torsional part of F; the linear-rotation part contributes a simple rigorously calculable factor to the matrix element in the coherent-state representation. (Note, incidentally, the interesting "complementarity" to the (J^2, J_z) -representation employed in the present paper: Here it is the torsional part that enjoys a simple rigorous form of its matrix element while the rotational part requires a semiclassical approximation.) The accuracy for the 2j + 1 eigenvalues of F was found to be about 3% of the mean spacing $2\pi/(2j + 1)$ of the eigenphases.

From a classical point of view the coherent states employed in Ref. [5] have the intuitive appeal that their span in the phase space shrinks to a point in the classical limit. However, this nice property actually makes for a drawback for the semiclassical behavior of matrix elements between two coherent states: No classical trajectory can in general be associated with such a matrix element simply because specifying both the initial and final phase-space points amounts to an overdetermination of the classical trajectory. As a consequence, the semiclassical Floquet matrix is built from contributions of "ghost trajectories", i.e. complex solutions of the real equations of motion, which are entities rather removed from classical reality [6, 7]. Nevertheless the excellent accuracy obtained for the spectrum in the limit of small $1/j \propto \hbar$ gives support to the expectation that chaotic as well as regular dynamical systems do allow for systematic semiclassical approximations for their spectra.

We here employ the 2j+1 angular-momentum eigenstates $|i,m\rangle$ with fixed i as a basis and semiclassically approximate the matrix elements $\langle j, m | F | j, m' \rangle$. As was explained in the foregoing sections the fraction $(\pi/4) \sin \beta$ of the total number $(2j + 1)^2$ of these matrix elements corresponds to classical trajectories. No overdetermination is incurred since by fixing the initial and final quantum numbers m_i, m_f we specify initial and final momenta for the classical trajectory. Only for pairs m_i, m_f outside the ellipse of Fig. 2 there are no classically permissible trajectories. Since these classically forbidden pairs amount only to the fraction $1 - (\pi/4) \sin \beta$ of all pairs one might expect that by working with the basis formed by the angular momentum eigenstates $|j, m\rangle$ one makes better use of classical reality than is possible with the coherent-state basis. Indeed, for all matrix elements corresponding to classically allowed trajectories these and only these solutions of the stationary-phase equations are needed to determine the semiclassical approximation; that approximation is then at least as easily implementable as the calculation of the quantum mechanically exact value of the matrix element. On the other hand, a lot more and harder work was necessary in the coherent-state basis, since the stationaryphase equation arising there for every matrix element has an infinity of ghost trajectories as solutions many of which may make quantitatively important contributions to the matrix element, while others must be discarded since they cannot be reached by allowable paths of integration. It is thus fair to say that diagonalizing the Floquet matrix after semiclassically approximating its elements in the (J^2, J_z) basis is an efficient strategy to establish the semiclassical quasienergy spectrum.

In order to ascertain the accuracy of the semiclassical spectrum we must compare it with the exact one. To that end we have also diagonalized the exact Floquet matrix $\langle j, m_f | F | j, m_i \rangle = e^{-ikm_f^2/2J} d_{m_f,m_i}(\beta)$ after numerically evaluating the matrix elements $d_{m_f,m_i}(\beta)$. An efficient way to do that for large j employs the well known recurrence relation [17]

$$d_{m_1 \pm 1, m_2}(\beta) = \frac{1}{f(\mp m_1)} \\ \times \left(\frac{m_2 - m_1 \cos \beta}{\sin \beta} d_{m_1, m_2} - f(\pm m_1) d_{m_1 \mp 1, m_2}\right)$$
(8.1)

where $f(m) = \frac{1}{2}\sqrt{(j+m)(j-m+1)}$. To minimize accumulation of numerical errors we had to use both starting points $d_{j,j}(\beta) = \left(\cos\frac{\beta}{2}\right)^{2j}$, $d_{-j,j}(\beta) = \left(\sin\frac{\beta}{2}\right)^{2j}$, and the symmetry properties (3.5).

Let us finally turn to our numerical results. The exact eigenvalues of F all lie on the unit circle in the plane of complex numbers, due to the unitarity of F. The semiclassical approximation slightly violates unitarity and thus gives rise to radial as well as phase errors, both of the order 1/j for large j. Errors of that order threaten, of course, to render useless calculations of lowest order in $\hbar \propto 1/j$ since the mean spacing between neighboring eigenphases, $2\pi/(2j+1)$, is of that very same order. It was in fact the principal result of Ref. [5] that the error is such a small fraction of the mean spacing that each approximate eigenvalue can be uniquely associated with its exact partner. We here recover such fine accuracy.

As quantitative measures of the errors incurred we employ the root mean squares of the deviations of (i) the moduli r_i^{SC} of the semiclassical eigenvalues from unity and (ii) the semiclassical quasienergies alias eigenphases ϕ_i^{SC} from their exact counterparts ϕ_i ,

$$\Delta r = \sqrt{\frac{1}{2j+1} \sum_{i=1}^{2j+1} (r_i^{\text{SC}} - 1)^2},$$

$$\Delta \phi = \sqrt{\frac{1}{2j+1} \sum_{i=1}^{2j+1} (\phi_i^{\text{SC}} - \phi_i)^2},$$
(8.2)

with the means taken over all 2j + 1 eigenvalues of a spectrum. We display these errors as functions of the quantum number j in Fig. 4. The first of them (Fig. 4a) pertains to vanishing torsion strength, k = 0, i. e. the case of a pure rotation by the angle $\beta = 1$ about the *y*-axis. Both the radial and



Fig. 4. Relative error of eigenphases (right column) and radii (left column) of the semiclassical eigenvalues for $\mathbf{a} \ \beta = 1$, k = 0, $\mathbf{b} \ \beta = \pi/2$, k = 1, and $\mathbf{c} \ \beta = \pi/2$, k = 8

the phase error turn out as roughly 1% of the mean spacing. Needless to say that in this fully integrable case the exact eigenphases are known explicitly as the eigenvalues of J_{μ} taken modulo 2π . Next, Fig. 4b gives the errors for the case $\beta = \pi/2$, k = 1 which is classically characterized by a mixed phase space with small chaotic islands and regular motion everywhere else. Again, the errors never exceed a few percent of the mean spacing in the range of j investigated; the slight growth with j might be a purely numerical artefact. Interestingly, the error incurred with the uniform WKB approximation for the linear rotation can be reduced by roughly a factor 2 by resorting to the harmonic-oscillator approximation (3.11) for the matrix elements with $m_i \approx \pm j$, $m_f \approx 0$ or $m_f \approx \pm j$, $m_i \approx 0$. It is also interesting to see that for this near integrable case the results previously obtained with the coherent-state basis are slightly superior to the ones advocated here; this is quite intuitive since the semiclassical treatment of linear rotation in the coherent-state basis is in fact rigorous [14] and since a torsion of strength k = 1 is

but a small perturbation of the linear rotation. As soon as we crank up the torsion strength k to secure predominance of chaos in the classical phase space we obtain better accuracy with the (\mathbf{J}^2, J_z) basis, as is revealed in Fig. 4c for the case k = 8, $\beta = \pi/2$: With the refinement provided by the harmonic-oscillator approximation mentioned above we get the quasienergies to within 1% of the mean spacing and the moduli even slightly better.

We gratefully acknowledge support by the Sonderforschungsbereich "Unordnung und große Fluktuationen" of the Deutsche Forschungsgemeinschaft, the International Science Foundation (Grant R21000), and the Russian Fundamental Research Fund (Grant No. 94-02-06022-a). We thank Marek Kuś, Bruno Eckhardt, and Eugene Bogomolny for helpful discussions.

Appendix A: Derivation of WKB asymptotics

The asymptotics of Wigner's *d*-functions in the limit of large angular momenta was originally obtained by solving their differential equation in the WKB approximation [10, 11]. We shall here sketch the less known but somewhat more economical WKB treatment of the recursion relations (8.1). For a more detailed presentation we refer to [8].

Momentarily simplifying the notation as $d_{m_f,m_i}^j \rightarrow d_{m_f}$ we write (8.1) in the form of a Hermitian three-step recurrence relation

$$p_m d_{m-1} + (w_m - E)d_m + p_{m+1}d_{m+1} = 0,$$
(A1)

where the eigenvalue E plays the role of the second index m_i ; the coefficients p_m , w_m may be read off from the original relation (8.1) as $w_m = m \cos \beta$ and $p_m = \frac{1}{2} \sin \beta [(j+m)(j-m+1)]^{\frac{1}{2}}$. We again extend the independent variable m from integer to continuous. To construct the asymptotic solution we assume the coefficients to depend but weakly on m and make the ansatz

$$d_m = A(m) \ e^{iS(m)} \tag{A2}$$

with slowly varying amplitude A and "action" S. In view of $p_m = O(j)$, $\partial p_m / \partial m = O(1)$ it is consistent to assume that the derivatives of the action and the amplitude have the weights $A^{(n)} = O(j^{-n})$, $S^{(n)} = O(j^{1-n})$. By expanding these functions as $S(m \pm 1) = S(m) \pm S'(m) + \frac{1}{2}S''(m)$ etc. we easily find, to lowest order in 1/j and up to a normalization factor,

$$d_m \approx d_m^{\text{WKB}} \propto \frac{1}{\left[2p_{m+\frac{1}{2}}\sin\phi\right]^{1/2}}\cos\left[\int_{m_0}^m \phi(n)dn + \theta_0\right]$$
(A3)

with the function

$$\phi(m) = \arccos \frac{E - w_m}{2p_{m+\frac{1}{2}}} \tag{A4}$$

determinig both the action, $S' = \phi$, and the prefactor; θ_0 is a constant to be determined below. As long as the function $\phi(m)$ is real, the solution (A3) oscillates. This is the case when the argument of the arccosine lies between -1 and 1 and characterizes the "classically allowed region" of the variable m; beyond that region one of the two fundamental solutions of the recursion relation grows exponentially while the other one decays. One can also speak about "turning points" of m separating classically allowed and forbidden regions. These are the values of m (not necessarily integer) which satisfy the equations $\phi(m) = 0$ and $\phi(m) = \pi$ and are commonly called the "usual" and "unusual" turning points, respectively.

Consider a usual turning point m_t and suppose that $\phi(m)$ is real to the right of m_t . It can be shown that within the allowed region the physically acceptable solution which matches to a decaying exponential for $m < m_t$ is obtained if we take $m_0 = m_t$ in (A3) and choose the phase as $\theta_0 = -\pi/4$. (For an unusual turning point the matching phase would read $\theta_0 = m_t \pi + \pi/4$.)

Suppose now that the classically allowed region of m is bounded on both sides by two turning points. The asymptotic

solution which decays both to the left and to the right of the allowed region exists only for discrete values of E which are the (asymptotic) eigenvalues of the recursion relation. The corresponding eigenvector $\{d_m\}$ can be normalized as $\sum_m d_m^2 = 1$.

There is a simple connection between the WKB solutions of recurrence relations and differential equations [18]. Indeed, the function $g(m) = (S'(m))^{-\frac{1}{2}}e^{iS(m)}$ obeys the differential equation

$$g''(m) + (S'(m))^2 g(m) = 0,$$
(A5)

provided one drops, with appeal to the slow variation in m and in the spirit of the WKB approximation, correction terms involving second and higher derivatives of S(m). We identify again $S'(m) = \phi(m)$. Then if m_t is a usual turning point of the recursion relation (A1) with the function $\phi(m)$ positive for $m > m_t$ and imaginary for $m < m_t$, the differential equation (A5) has that same turning point, with classically allowed and forbidden regions situated at $m > m_t$ and $m < m_t$, respectively. Within the classically allowed region (A5) has the WKB solution matched with the solution decreasing outside,

$$g^{\text{WKB}}(m) \propto \frac{1}{[\phi(m)]^{1/2}} \cos\left(\int_{m_t}^m \phi(n') dn' - \pi/4\right).$$
 (A6)

Comparing (A6) and (A3) we see that the semiclassical asymptotics of the recurrence relation and the differential equation are related by

$$d_m^{\mathbf{WKB}} = \sqrt{\frac{\phi(m)}{\sin\phi(m)}} g^{\mathbf{WKB}}(m).$$
(A7)

The connection just established allows to construct an improved WKB solution of the recurrence relation which does not diverge at the turning point. We simply have to invoke the well known uniform WKB solution of the differential equation (A5) which remains valid in the vicinity of the turning point and provides a smooth interpolation between the semiclassical approximations in the classically allowed and forbidden regions (cf. [19, 10.4.111-116]),

$$g^{\text{unif}}(m) = \left[\frac{\xi(m)}{\phi^2(m)}\right]^{1/4} \operatorname{Ai}\left(\lambda(m)\right).$$
(A8)

Here Ai (λ) is the Airy function. Its argument,

$$\lambda(m) = -\left(\frac{3}{2} \int_{m_t}^m \phi dn\right)^{2/3}, \qquad m > m_t,$$

$$\lambda(m) = \left(\frac{3}{2} \int_m^{m_t} |\phi| dn\right)^{2/3}, \qquad m < m_t,$$
 (A9)

is a smooth monotonically growing function of m passing through zero in the turning point. By replacing in the r.h.s. of (A7) the primitive WKB solution g^{WKB} of the differential equation (A5) by its more sophisticated version g^{unif} , we obtain the desired improvement of the semiclassical solution of the recurrence relation. Actually, this is true only if m_t is a usual turning point since for $\phi(m_t) = \pi$ the transformation (A7) becomes singular. The case of an unusual turning point is treated by substituting $d_m \rightarrow (-1)^m d_m$ in the recurrence relation (A1) whereupon m_t becomes a usual turning point.

Up to here our reasoning has not made use of the special form of the coefficients p_m, w_m pertaining to Wigner's *d*-function. Invoking these forms we recover the result extensively used in the main body of the paper, i. e. (3.1,3.2) for the *d*-function and the turning points in accord with the previously encountered classically allowed elliptic region (3.3). In a similar way, the above connection (A7) with gWKB taken as the uniform asymptotic solution of the differential equation (A5) leads to the uniform asymptotics (3.7) of the *d*-function.

The foregoing asymptotic analysis rests on the formal assignment of orders in $\hbar \propto 1/j$ as $p_m = O(j)$, $p'_m = O(1)$ and therefore breaks down when m approaches the values $\pm j$; in that range the coefficient p_m ceases to vary slowly with m and the WKB approximation looses its validity. A similar failure is observed if it is m_i which tends to its extremal values $\pm j$ whereupon the turning points move close to one another. This is analogous to the well-known inapplicability of the WKB method to the ground states of quantum systems.

We must worry about the inadaequacy of the WKB approximation just mentioned when the point in the m_f - m_i -plane defined by the subscripts m_f, m_i of the *d*-function is close to one of the tangency points between the ellipse bounding the classically allowed region and the square $|m_f| = J, |m_i| = J$ (Fig. 2). There are four such points; however due to the symmetry conditions (3.5) it is sufficient to consider, say, the one corresponding to $m_f = J \cos \beta$, $m_i = J$. In its vicinity the *d*-functions change slowly with each step of the recursion relation (8.1). This can be inferred from the fact that the function $\phi(m_f)$ determining the increment of the phase of the WKB solution (A3) is almost zero in this area. Therefore we can replace the finite differences in (8.1) by Taylor expansions as

$$d_{m_f \pm 1, m_i}^j \approx \left(1 \pm \frac{\partial}{\partial m_f} + \frac{1}{2} \frac{\partial^2}{\partial m_f^2} \right) d_{m_f, m_i}^j.$$
(A10)

We similarly expand the off-diagonal coefficients in (8.1) in powers of $m_f - J \cos \beta$ and employ

$$\sin \beta \sqrt{J^2 - m_f^2} \approx J \sin^2 \beta - \cos \beta$$
$$\times (m_f - J \cos \beta) - \frac{(m_f - J \cos \beta)^2}{2J \sin^2 \beta}$$
(A11)

for the coefficient of d_{m_f,m_i}^j while leaving only the zerothorder term in the coefficient of the derivatives of the *d*function (An estimate of errors introduced by this type of approximation and the higher-order corrections can be found in [9]). By finally changing notations as

$$n = j - m_i, \quad x = \frac{m_f - J \cos\beta}{\sqrt{J \sin^2 \beta}},$$

$$\psi_n(x) = \sqrt[4]{J \sin^2 \beta} d^j_{m_f, j-n}$$
(A12)

we turn the recursion relation for d_{m_f,m_i}^j into Schrödinger's equation for the harmonic oscillator,

$$-\frac{1}{2}\frac{d^2\psi_n}{dx^2} + \frac{x^2}{2}\psi_n(x) = \left(n + \frac{1}{2}\right)\psi_n(x).$$
 (A13)

By normalizing that state to unity we recover the desired harmonic-oscillator approximation for the properly normalized *d*-functions with m_i close to *j*.

References

- F. Haake, M. Kuś, R. Scharf: In F. Haake, L. M. Narducci, D. F. Walls (eds.): *Coherence, Cooperation, and Fluctuations*, Cambridge University Press, Cambridge (1986)
- 2. F. Haake, M. Kuś, R. Scharf, Z. Phys. B 65, 381 (1987)
- 3. H. Frahm, H. J. Mikeska: Z. Phys. B 60, 117 (1985)
- 4. F. Haake, Quantum Signatures of Chaos, Springer, Berlin (1991)
- P. Gerwinski, F. Haake, M. Kuś, H. Wiedemann, K. Życzkowski, Phys. Rev. Lett. 74, 1562 (1995)
- 6. M. Kuś, F. Haake, D. Delande, Phys. Rev. Lett. 71, 2167 (1993)
- R. Balian, G. Parisi, A. Voros, Phys. Rev. Lett. 41, 1141 (1978); R. Balian, in: Discourses in Mathematics and its Applications, No. 1, Eds. S. A. Fulling, F. J. Narcovich, Dept of Mathematics, Texas A&M University, College Station, Texas (1991)
- 8. P. A. Braun, Rev. Mod. Phys. 65, 115 (1993).
- 9. P. A. Braun, Opt. Spectrosc. (USSR) 66, 32 (1989)
- 10. P. Brussard, H. Tolhoek, Physica 23, 955 (1957).
- P. Ponzano, T. Regge, in *Spectroscopic and Group Theoretical Methods in Physics*, edited by F. Bloch, S. G. Cohen, A. De-Schalit, S. Sambursky, I. Talmi (Wiley, New York), p.53
- 12. W. M. Miller, Adv. Chem. Phys. 25, 69 (1974)
- L. C. Biedenharn, J. D. Louck, *The Racah-Wigner Algebra in Quantum Theory* (Encyclopedia of Mathematics and Its Applications, Volume 9, Addison-Wesley, 1981)
- 14. M. Kuś, F. Haake, B. Eckhardt, Z. Phys. B 92, 221 (1993)
- 15. G. Junker, H. Leschke, Physica D 56, 135 (1992)
- 16. Actually, the trace formula of [14] contains a phase factor for which no semiclassical explanation could be given. That phase factor does not arise for the new definition of the Floquet operator F given in (1.1), due to the semiclassically more appropriate scaling of the torsion generator.
- D. A. Varŝaloviĉ, Kvantovaja teorija uglovogo momenta, Singapore, World Scientific (1988)
- 18. K. Schulten, R. G. Gordon, J. Math. Phys. 16, 1971 (1975)
- M. Abramowitz, I. A. Stegun: Handbook of mathematical functions, Dover Publications, inc., New York, 1965