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Closed Orbits and Semiclassical Wavefunctions in Two-Dimensional Hamiltonian Systems

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The periodic-orbit theory of the density-of-states and the closed-orbit theory of atomic absorption spectra relate properties of a quantum system to properties of periodic or of closed orbits of a system. In these theories, every return of an orbit to the initial point makes a contribution, so in general for each orbit an infinite number of terms must be computed and summed. We show that the term asising from the nth return of an orbit can be calculated from properties of the orbit on its first return.

KEY WORDS: Semiclassical approximation; Green's function; closed-orbit theory; Maslov index; atomic absorption spectra.

1. BACKGROUND

Semiclassical descriptions of quantum mechanical systems often begin with a semiclassical approximation to the Green function $G_E(\mathbf{q}, \mathbf{q}')$. For example, the periodic-orbit theory of the quantum density of states starts from this point.[(1)] Similarly, the closely-related closed-orbit theory of atomic absorption spectra describes waves which propagate away from and later return to an atom.[(2)] The waves described in this theory can be regarded as a kind of generalized Green function.

The conventional Green function $G_E(\mathbf{q}, \mathbf{q}')$ represents waves that arise at $\mathbf{q}$ from a steady point source that sends out waves of fixed energy uniformly in all directions. In the generalized Green function, which we denote $F_E(\mathbf{q}, \mathbf{q}')$, the waves still have fixed energy, but the source sends them out with some specified initial angular distribution, such as a p wave, or some combination of s and d waves.

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In both theories we are concerned with waves that propagate outward from and later return to the source point. The density of states is proportional to the trace of the Green function $\int G_E(\mathbf{q}, \mathbf{q})\, d\mathbf{q}$, while an atomic absorption cross section is proportional to an integral of G_E with a very localized source function $\int \psi_s(\mathbf{q})\, G_E(\mathbf{q}, \mathbf{q}')\, \psi_s(\mathbf{q}')\, d\mathbf{q}\, d\mathbf{q}'$. The source function is so localized that the relevant quantity is the generalized Green function evaluated at the source point, $F_E(\mathbf{q}, \mathbf{q})$.

The semiclassical approximations to $G_E(\mathbf{q}, \mathbf{q})$ and $F_E(\mathbf{q}, \mathbf{q})$ involve classical trajectories that begin and end at the point $\mathbf{q}$—closed orbits. Now in a typical system, a closed orbit goes out from $\mathbf{q}$ in one direction, returns to $\mathbf{q}$ from another direction, and then goes out again, perhaps never to return. Most such orbits are not relevant to the density of states. When a stationary-phase approximation is used to evaluate the trace of G, one finds that only periodic orbits contribute.

For atomic absorption spectra, not only periodic orbits, but also closed orbits contribute. However, the Coulomb field has a special property which brings periodicity back into the system. When a classical electron is incident on a fixed positive charge at zero impact parameter, the Coulomb field scatters the electron back exactly in the direction from which it came. It follows that orbits which are closed at the nucleus with return time T retrace themselves such that they are periodic with period $2T$.

In either case, then, the functions $G_E(\mathbf{q}, \mathbf{q})$ and $F_E(\mathbf{q}, \mathbf{q})$ involve repeated returns to the source point. The semiclassical approximation to either function has the form

$$\sum_k \sum_n B_{kn} e^{i(S_{kn}/\hbar - \mu_{kn}\pi/2)}$$

The index k labels a particular "primitive" closed orbit, while n labels the repetitions of that orbit. S_{kn} is the classical action on the nth return of the kth closed orbit, B_{kn} is an amplitude, and μ_{kn} is the associated Maslov index.

Question: Can we find the amplitude B_{kn} and the Maslov index μ_{kn} for all repetitions n from properties of the closed orbit on its first return? If such formulas can be found, they would greatly simplify the numerical calculations that are required for implementation of periodic-orbit theory and closed-orbit theory.

This question was first addressed by Guttzwiller in a slightly different manner.[1] Writing the trace of G_E as $\sum_{k,n} C_{kn} \exp i(S_{kn}/\hbar - \sigma_{kn}\pi/2)$, he gave formulas for C_{kn} and stated that $\sigma_{kn} = n\sigma_{k1}$. The result is not at all trivial, and was only recently proved by Creagh *et al.*[3] for unstable periodic orbits.[2] We need analogous results which apply to the Green function itself, which apply either to stable orbits or to unstable orbits, and which apply to closed orbits as well as to periodic orbits.

We are pleased to report that very simple formulas for B_{kn} and μ_{kn} can be written down, and that the formulas are easy to implement numerically. The results are stated in the following section after more precise definitions are given. Proofs are given in appendices. In Section 3 we explain how the results can be applied in calculations of atomic absorption spectra using the closed-orbit theory. The results can also be used in many other contexts, since our proofs are quite general. The important assumptions are as follows:

(i) The system has two degrees of freedom.

(ii) The Hamiltonian has the standard kinetic plus potential form, with H an even function of momenta.

(iii) The potential energy is smooth.

For application to closed-orbit theory, an additional assumption is involved:

(iv) The potential energy has two reflection symmetries.

2. MAIN RESULTS

2.1. Preliminary Definitions

Our particle moves in a two-dimensional "Cartesian" coordinate space (u, v), with

$$H = \frac{1}{2m}(p_u^2 + p_v^2) + V(u, v)$$

where $V(u, v)$ is a smooth function having no singularities. The source of particles is taken to be the origin of coordinates, and we define cyclindrical coordinates (R, Θ) in the usual way.

A fundamental quantity in closed-orbit theory[(2)] is a function that we denote $F_E(\mathbf{q}, \mathbf{0})$,

$$F_E(\mathbf{q}, \mathbf{0}) = \int G_E(\mathbf{q}, \mathbf{q}')\, \psi_s(\mathbf{q}')\, d\mathbf{q}'$$

where $\psi_s(\mathbf{q}')$ is a "source function," whose most important property is that it is a very localized function of $\mathbf{q}'$, practically zero outside of a small region

[2] A related study was done by Eckhardt and Wintgen.[(4)]

near the origin. For $\mathbf{q}$ outside the domain in which the source function is significant, this function $F_E(\mathbf{q}, \mathbf{0})$ is the generalized Green function. It contains outgoing waves with an angular distribution related to that of the source function, and in addition it contains returning waves that are correlated with closed orbits.

The initial outgoing wave is denoted $\psi^{\text{out}}(\mathbf{q})$ or $F^{\text{out}}(\mathbf{q}, \mathbf{0})$, and the returning wave associated with the nth return of the kth closed orbit is denoted $\psi_n^{\text{ret}}(\mathbf{q})$ or $F_n^{\text{ret}}(\mathbf{q}, \mathbf{0})$. In semiclassical approximation this quantity is given by

$$\psi_n^{\text{ret}}(\mathbf{q}) = A_n(\mathbf{q}, \mathbf{q}_0)\{\exp i[S_n(\mathbf{q}, \mathbf{q}_0)/\hbar - \mu_n \pi/2]\partial \psi^{\text{out}}(\mathbf{q}_0)$$

Everything in this formula should be decorated with the label k of the closed orbit, but henceforth we consider any one particular orbit and drop that label. $\mathbf{q}_0$ means (R_0, Θ_i): the outgoing wave is evaluated on a small circle near the origin at an angle Θ_i which is the initial outgoing direction of the closed orbit; $\psi^{\text{out}}(R_0, \Theta_i)$ is the outgoing wave in that direction. $S_n(\mathbf{q})$ is the classical action integrated along the trajectory that arrives at $\mathbf{q}$ starting from $\mathbf{q}_0$,

$$S_n(\mathbf{q}) = \int_{\mathbf{q}_0}^{\mathbf{q}} \mathbf{p} \cdot d\mathbf{q}$$

A_n is the "classical amplitude" of the returning wave (the square root of the classical density).

2.2. The Classical Amplitude and a Poincaré Map

Given a closed orbit which starts from the circle at angle Θ_{i} and return at $\Theta_{\text{f}}(1)$, the orbit continues through the origin, and its successive returns occur at $\Theta_{\text{f}}(n)$. Now suppose we change the initial angle to $\Theta_{\text{i}} + d\Theta_{\text{i}}$, and compute the trajectory until its nth return to the circle. It final angle is $\Theta_{\text{f}}(n) + d\Theta_{\text{f}}(n)$.

The amplitude A_n can be expressed in terms of the rate of change of the returning angle with respect to the initial lauching angle,

$$A_n = \left| \frac{\partial \Theta_{\text{f}}(n)}{\partial \Theta_{\text{i}}} \right|^{-1/2} \tag{2.1}$$

The proof is given in Appendix A.

The angular derivative can be further expressed in terms of elements of the linear stability matrix about the closed orbit.[3] Let us presume

[3] The relationship between the classical amplitude and a matrix element of the monodromy matrix was first pointed out to one of us by J. Main.

that the orbit passes transversely through $u=0$, and we take a Poincaré surface of section at $u=0$, and define a Poincaré map on the surface, $(v_0, p_{v0}) \rightarrow (v_1, p_{v1})$. In phase space we start at $u_0=0$, with arbitrary v_0 and p_{v0} and set $p_{u0}>0$ using the fixed value of the Hamiltonian. We then integrate Hamilton's equations of motion forward in time through one cycle of the orbit until $u=0$ and $p_u>0$, and record the values of v_1 and p_{v1}. This map is the conventional Poincaré map. (In the closed-orbit theory of atomic absorption spectra, the potential energy has symmetries such that it is better to stop whenever $u=0$ regardless of the sign of p_u.[5] The following formulas apply also to this unconventional Poincaré map.) Let (v_n, p_{vn}) be $(v(t), p_v(t))$ at the nth return to $u=0$ from the initial conditions (v_0, p_{v0}). The Jacobian matrix of the linearized map about the closed orbit is written as

$$\mathbf{J}(n) \equiv \begin{pmatrix} \dfrac{\partial v_n}{\partial v_0} & \dfrac{\partial v_n}{\partial p_{v0}} \\ \dfrac{\partial p_{vn}}{\partial v_0} & \dfrac{\partial p_{vn}}{\partial p_{v0}} \end{pmatrix}_{u=0,\, n\text{th return}} \equiv \begin{pmatrix} J_{11}(n) & J_{12}(n) \\ J_{21}(n) & J_{22}(n) \end{pmatrix}$$

The matrix element $J_{12}(n)$ is related to the angular derivative by

$$\frac{\partial \Theta_{\mathrm{f}}(n)}{\partial \Theta_{\mathrm{i}}} = \frac{m\dot{R}_{\mathrm{i}}}{R_0} \cos \Theta_i \cos \Theta_{\mathrm{f}}(n)\, J_{12}(n) \tag{2.2}$$

where $\dot{R}_{\mathrm{i}}$ is the initial outgoing speed of the particle. The proof is given in Appendix B. Combining Eqs. (2.1) and (2.2), we can express the amplitude of the semiclassical wavefunction in terms of $J_{12}(n)$.

In the following we will relate $J_{12}(n)$ and μ_n to properties of the orbit on its first return. The three quantities that are required are $J_{12}(1)$, $T_1 = \mathrm{Tr}\, \mathbf{J}(1)$, and μ_1, the Maslov index on the first return.

2.3. The Classical Amplitude for Repetitions of Periodic Orbits

In general the Jacobian matrix for the nth closure is related to matrices for single closures by

$$\mathbf{J}(n) = \frac{\partial(v_n, p_{vn})}{\partial(v_0, p_{v0})} = \frac{\partial(v_n, p_{vn})}{\partial(v_{n-1}, p_{vn-1})} \frac{\partial(v_{n-1}, p_{vn-1})}{\partial(v_{n-2}, p_{vn-2})} \cdots \frac{\partial(v_1, p_{v1})}{\partial(v_0, p_{v0})}$$

Each of these Jacobian matrices is a function of the coordinates (v, p_v) spanning the surface of section. For any orbit it is always the same function of two variables, but it is evaluated at the distinct points where the orbit crosses the surface. For closed orbits the point is always $v=0$, but p_v could vary with each closure.

Now suppose the closed orbit is periodic, with period 1 (every time the orbit returns to the origin, the final momentum equals the initial momentum). Then each of the factors in the equation above is evaluated at the same point, so each is the same matrix, $\mathbf{J}(1)$, which we will simply denote $\mathbf{J}$ henceforth. Therefore

$$\mathbf{J}(n)=\mathbf{J}^n \qquad \text{for periodic orbits}$$

The map is area-preserving, so $\det(J)=1$. Let the eigenvalues of $\mathbf{J}(n)$ be written as $\exp(\pm i\alpha_n)$ if the orbit is stable, or $\pm\exp(\pm\beta_n)$ if it is unstable. [The two eigenvalues are $\exp(\beta)$ and $\exp(-\beta)$ if $\mathrm{Tr}\,\mathbf{J}(n)\geqslant 2$ (hyperbolic point) or they are $-\exp(\beta)$ and $-\exp(-\beta)$ if $\mathrm{Tr}\,\mathbf{J}(n)< -2$ (hyperbolic with reflection).] α_n is the winding angle on the surface of section, and β_n is the Lyapunov exponent. Clearly $\alpha_n=n\alpha_1$ and $\beta_n=n\beta_1$.

The formulas below depend upon a specific convention involving α_1: We choose $0\leqslant\alpha_1<\pi$ (and $\beta_1>0$).

For any 2×2 matrix having determinant equal to 1,

$$|[\mathbf{J}^n]_{12}|=|J_{12}|\left|\frac{T_n^2-4}{T_1^2-4}\right|^{1/2} \qquad \text{if} \quad \mathrm{Det}\,\mathbf{J}=1 \tag{2.3a}$$

where J_{12} is $J_{12}(1)$, and T_n is the trace of $\mathbf{J}_n$,

$$T_n\equiv\mathrm{Tr}\,\mathbf{J}_n=\begin{cases}2\cos(n\alpha_1), & \text{stable}\\ 2\cosh(n\beta_1), & \text{unstable}\\ (-)^n 2\cosh(n\beta_1), & \text{unstable with reflection}\end{cases} \tag{2.3b}$$

$[J^n]_{12}$ can also be expressed in terms of α_1 and β_1 as

$$[\mathbf{J}^n]_{12}=\begin{cases}J_{12}\dfrac{\sin(n\alpha_1)}{\sin\alpha_1}, & \text{stable}\\[2ex] J_{12}\dfrac{\sinh(n\beta_1)}{\sinh\beta_1}\dfrac{\mathrm{sgn}(T_n)}{\mathrm{sgn}(T_1)}, & \text{unstable}\end{cases} \tag{2.3c}$$

These results are proved in Appendix C.

Equations (2.3a) and (2.3b), combined with Eqs. (2.1) and (2.2), allow us to evaluate the amplitude A_n on the nth return from properties of the matrix $\mathbf{J}$ on the first return. Specifically, from $J_{12}(1)$, T_1, and μ_1 we compute α_1 or β_1, from that we compute T_n, and then we obtain $|J_{12}(n)|$.

4. MASLOV INDEX FOR REPETITIONS OF PERIODIC ORBITS

The Maslov index for the nth repetition of a periodic orbit is n times the Maslov index for the first return plus an integer we call ν_n,

$$\mu_n = n\mu_1 + \nu_n \tag{2.4a}$$

If the orbit is stable,

$$\nu_n = \begin{cases} \mathrm{Int}(n\alpha_1/\pi), & J_{12} > 0 \\ \mathrm{Int}[n(\pi - \alpha_1)/\pi], & J_{12} < 0 \end{cases} \tag{2.4b}$$

If the orbit is unstable,

$$\nu_n = \begin{cases} 0, & J_{12}\,\mathrm{Tr}\,\mathbf{J} > 0 \\ n-1, & J_{12}\,\mathrm{Tr}\,\mathbf{J} < 0 \end{cases} \tag{2.4c}$$

These formulas require the previous mentioned convention on α_1. Four Appendices (D–G) are needed to prove these simple results.

Using Eqs. (2.1)–(2.3), we can express the semiclassical wavefunction associated with a periodic orbit and its repetitions as

$$\psi^{\mathrm{ret}}(R_0, \Theta_f) = \psi^{\mathrm{out}}(R_0, \Theta_i) \left| \frac{\partial \Theta_f(1)}{\partial \Theta_i} \right|^{-1/2} \times \sum_{n=1}^{\infty} \begin{cases} \left| \dfrac{\sin \alpha_1}{\sin(n\alpha_1)} \right|^{1/2} e^{in(S_1/\hbar - \mu_1\pi/2) - i\nu_n\pi/2}, & \text{stable} \\ \left(\dfrac{\sinh \beta_1}{\sinh(n\beta_1)} \right)^{1/2} e^{in(S_1/\hbar - \mu_1\pi/2) - i\nu_n\pi/2}, & \text{unstable} \end{cases} \tag{2.5a}$$

or, in terms of the trace T_1,

$$\psi^{\mathrm{ret}}(R_0, \Theta_f) = \psi^{\mathrm{out}}(R_0, \Theta_i) \left| \frac{\partial \Theta_f(1)}{\partial \Theta_i} \right|^{-1/2} \sum_{n=1}^{\infty} \left[\left| \frac{T_1^2 - 4}{T_n^2 - 4} \right|^{1/4} e^{in(S_1/\hbar - \mu_1\pi/2) - i\nu_n\pi/2} \right] \tag{2.5b}$$

Here the phase of the wavefunction has two terms. The first term, $n(S_1/\hbar - \mu_1\pi/2)$, is simply the n multiple of the phase for the first return. The second terms is $\nu_n\pi/2$, where ν_n is given by Eq. (2.4).

2.5. Repetition of Closed Orbits in a System with Reflection Symmetries

We now assume that the potential energy $V(u, v)$ has two reflection symmetries, $V(\pm u, \pm v) = V(u, v)$, and we consider orbits that are closed at the origin. The symmetries ensure that any orbit which returns to the origin at time T_c is periodic with period $T_p = 2T_c$. As mentioned earlier, it is convenient to define a Poincaré "half-map" $(v_0, p_{v0}) \rightarrow (v_1', p_{v1}')$ in which the integration is stopped when $u = 0$ near the closure time T_c. We let $\mathbf{J}(1)$ be the Jacobian matrix of this half-map, and S_1 and μ_1 be the classical action and Maslov index at the closure time.

The closed orbits can be classified as two types (see Fig. 1). In type 1, $|p_{v0}| = |p_{v1}|$. Two cases arise. If $p_{v0} = p_{v1}$, then a picture of the orbit in configuration space has two reflection symmetries, and this closed orbit of the differential equations is a periodic orbit of the half-map. If $p_{v0} = -p_{v1}$, then the orbit has inversion symmetry, but not reflection symmetry. Such orbits have endpoints where the particle stops and retraces its path. Orbits of type 2 have inversion symmetry but not reflection symmetry, and there is no relationship between p_{v0} and p_{v1}.

For the first type of orbit, all the results of the previous section apply without any change. Repetitions of a closure are effectively the same as repetition of a period. However, for the second type, the second closure is similar to the first closure in reverse. In Appendices H and I we show that the Jacobian matrix for the second closure is related by $\mathbf{J}_1$ by

$$\frac{\partial(v_2, p_{v2})}{\partial(v_1, p_{v1})} = \begin{pmatrix} J_{22} & J_{12} \\ J_{21} & J_{11} \end{pmatrix} \equiv \mathbf{J}', \qquad \text{type 2 orbits} \tag{2.6a}$$

Note that the diagonal elements are exchanged. Since two closures equal one period, the Jacobian matrix for the third run, $\partial(v_3, p_{v3})/\partial(v_2, p_{v2})$, is $\mathbf{J}$ again, and

$$\mathbf{J}_n = \cdots \mathbf{J}\,\mathbf{J}'\,\mathbf{J}\,\mathbf{J}'\,\mathbf{J} \tag{2.6b}$$

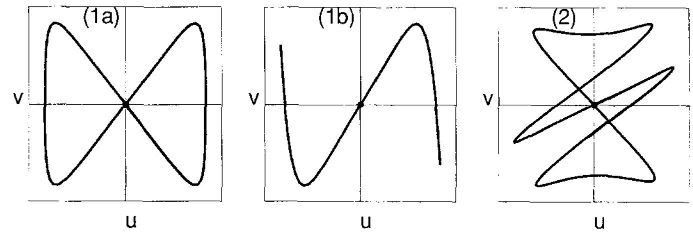

Fig. 1. Two types of orbits closed at the origin in a system with two reflection symmetries. In type 1, $|p_{v0}| = |p_{v1}|$. In type 1a, $p_{v0} = p_{v1}$. In type 1b, $-p_{v0} = p_{v1}$. In type 2, $|p_{v0}| \neq |p_{v1}|$. For type 1 orbits $J_{11} = J_{22}$, while for type 2 orbits $J_{11} \neq J_{22}$. Also, in type 1 orbits, the period of the transverse force constant $k_\sigma(t)$ [Eq. (D14b)] equals the closure time of the orbit (half the period of the orbit), while in type 2 orbits, the period of $k_\sigma(t)$ equals the period of the orbit. (In this figure, u is the horizontal axis and v is the vertical axis.)

For such orbits we define α_1' such that

$$\cos\alpha_1' = s'(J_{11}J_{22})^{1/2}, \qquad s' \equiv \operatorname{sgn}(J_{11}+J_{22}), \qquad \text{if} \quad 0 < J_{11}J_{22} < 1$$
$$\cos(2\alpha_1') = s(2J_{11}J_{22}-1), \qquad s \equiv \operatorname{sgn}(J_{11}J_{22}), \qquad \text{otherwise} \tag{2.7a}$$

where α_1' is real with $0 < \alpha_1' < \pi$ if $0 < J_{11}J_{22} < 1$, and α_1' is pure imaginary otherwise. We further define a tracelike quantity T':

$$T_1' = s2\cos\alpha_1', \qquad T_n' = s2\cos(n\alpha_1') \tag{2.7b}$$

We show in Appendix J that the magnitude of $J_{12}(n)$ is

$$|J_{12}(n)| = \begin{cases} |J_{12}| \left(\dfrac{T_n'^2 - 4}{T_1'^2 - 4}\right)^{1/2}, & n \text{ odd} \\ |J_{12}| \left(\dfrac{T_n'^2 - 4}{T_1'^2 - 4}\right)^{1/2} \left|\dfrac{J_{22}}{J_{11}}\right|^{1/2}, & n \text{ even} \end{cases} \qquad \text{type 2 orbits} \tag{2.8}$$

In Appendix K we derive a formula for the Maslov indices of these orbits, $\mu_n = n\mu_1 + \nu_n$, where ν_n is defined below. Then, combining all results, we can express the returning semiclassical wavefunction at (R_0, Θ_f) as

$$\psi^{\text{ret}}(R_0, \Theta_f) = \psi^{\text{out}}(R_0, \Theta_i) \left|\frac{\partial\Theta_f(1)}{\partial\Theta_i}\right|^{-1/2} \times \left[\sum_{n\text{ odd}} + \left|\frac{J_{11}}{J_{22}}\right|^{1/4} \sum_{n\text{ even}}\right] \left|\frac{T_1'^2 - 4}{T_n'^2 - 4}\right|^{1/4} e^{in(S_1/\hbar - \mu_1\pi/2) - i\nu_n\pi/2} \tag{2.9}$$

where

$$\nu_n = \begin{cases} \operatorname{Int}(n\alpha_1'/\pi), & J_{12} > 0 \\ \operatorname{Int}[n(\pi - \alpha_1')/\pi], & J_{12} < 0 \end{cases} \; 0 < J_{11}J_{22} < 1$$
$$\qquad \begin{cases} 0, & J_{12}J_{22} > 0 \\ n - 1, & J_{12}J_{22} < 0 \end{cases} \; J_{11}J_{22} > 1 \tag{2.10}$$
$$\qquad \begin{cases} \operatorname{Int}[(n-1)/2], & J_{12}J_{22} > 0 \\ \operatorname{Int}(n/2), & J_{12}J_{22} < 0 \end{cases} \; J_{11}J_{22} < 0$$

Proof of Eq. (2.10) is given in Appendices J and K.

3. APPLICATIONS TO THE ATOMIC ABSORPTION SPECTRUM PROBLEM

The theory discussed in the previous section is for two-dimensional Hamiltonian systems with a potential energy whose angular dependence becomes negligible near the origin. The atomic absorption spectrum problem, however, is three-dimensional and has a Hamiltonian with a singularity at the origin. However, in many cases the polar angle ϕ is separable, and the standard regularization using semiparabolic coordinates eliminates the singularity at the origin. After this is done, the formulas in Section 2 can be used.

3.1. Regularization of Two-Dimensional Coulomb Problems

We begin from a Hamiltonian written in cylindrical coordinates (ρ, z); the Hamiltonian is presumed to be given in the form

$$H = \frac{1}{2m}(p_\rho^2 + p_z^2) - \frac{1}{(\rho^2 + z^2)^{1/2}} + U(\rho, z) = E$$

The function $U(\rho, z)$ is presumed to be smooth and nonsingular for all finite (ρ, z). It is originally defined for positive ρ, but we extend it to negative ρ with the convention $U(-\rho, z) = U(\rho, z)$. This Hamiltonian has a singularity at the origin. The polar angle in (ρ, z) space is denoted θ: $\theta = \tan^{-1}(\rho/z)$, $0 < \theta < \pi$.

Define semiparabolic coordinates $u = r^{1/2}\cos(\theta/2)$ and $v = r^{1/2}\sin(\theta/2)$ and a new independent variable $\tau(t)$ such that $d\tau/dt = 1/r(t)$. Then the new classical Hamiltonian becomes

$$\begin{aligned} H &= \frac{1}{2m}(p_u^2 + p_v^2) + V(u, v) = 2 \\ V(u, v) &= -E(u^2 + v^2) + (u^2 + v^2)\, U(\rho(u, v), z(u, v)) \end{aligned} \tag{3.1}$$

This transformation eliminates the Coulomb singularity, leaving a smooth potential energy. This potential energy is originally defined only in the positive quadrant $u > 0$, $v > 0$, but it can be extended into other quadrants, and it has two reflection symmetries

$$V(-u, v) = V(u, -v) = V(u, v) \tag{3.2}$$

which imply an inversion symmetry

$$V(-u, -v) = V(u, v) \tag{3.3}$$

In (u, v) space, the leading term in $V(u, v)$ is $-E(u^2 + v^2)$ near the origin, so the angular dependence of $V(u, v)$ is negligible. All formulas given in Section 2 are applicable. Note that the polar angles in (ρ, z) or (u, v) space are related by $\Theta = \theta/2$.

3.2. Focusing Effects Associated with (ρ, z) Coordinates and with the Coulomb Singularity

The Hamiltonian in the atomic absorption problem is actually three-dimensional and has a singularity at the origin. This will affect the counting of the Maslov index in the following ways.

(i) The z axis itself constitutes a focus. Every time an orbit in (ρ, z) space passes through the z axis, the Maslov index increases by 1.

(ii) The Coulomb center provides another focusing effect. Every time an orbit in (ρ, z) space returns to the nucleus and scatters back on itself, the Maslov index for the scattered Coulomb wave increases by 2. This holds for all orbits that return with $\theta_f \neq 0$. For returning orbits that lie exactly on the z axis ($\theta_f = 0$), the increase of the Maslov index for the scattered wave is 1. These rules were proved in ref. 6.

These two rules can be stated in (u, v) space as follows. Every time an orbit passes through either the u axis or the v axis, the Maslov index increases by 1. If it passes through the origin, it is usually passing throuogh both u and v axes, so the Maslov index increases by 2. However, if it lies exactly along the u axis or the v axis, then when it passes through the origin it is passing through only one axis, so the Maslov index increases by 1.

Taking into account the two rules states above, the full Maslov index in a three-dimensional Coulomb problem is

$$\mu_n = n\mu_1 + \nu_n + 2(n-1), \qquad \theta_f \neq 0 \tag{3.4a}$$

where μ_1 is the Maslov index for the first return, and includes visible caustics and the number of z-axis crossings, and ν_n is given by Eq. (2.10).

The orbit lying on the z axis is special in three ways. (1) Like all orbits of type 1b, it has an endpoint, which adds 1 to the Maslov index on each return (Appendix L). (2) As stated above, each passage through the nucleus adds 1 to the Maslov index of the following return. (3) Each time a neighbor of this orbit passes through it (a) the Maslov index increases by 1 because the neighbor is crossing the orbit, and (b) the Maslov index increases by another 1 because the neighbor is crossing the z axis. Hence the total change in the Maslov index is 2 for each such passage. After this double-counting is incorporated into μ_1, then for the zero-degree orbit we have

$$\mu_n = n\mu_1 + 2\nu_n + (n-1), \qquad \theta_f = 0 \tag{3.4b}$$

The argument is given in Appendix M.

3.3. Returning Wave

We now let our coordinate $\mathbf{q}$ mean (r, θ, ϕ) or (ρ, z, ϕ). Then the returning wavefunction associated with a particular closed orbit is

$$\psi^{\text{ret}}(\mathbf{q}) = \psi^{\text{out}}(\mathbf{q}_0) \left|\frac{\partial\theta_\text{f}}{\partial\theta_\text{i}}\right|^{-1/2} \left|\frac{\sin\theta_\text{i}}{\sin\theta_\text{f}}\right|^{1/2} \times\left[\sum_{n\text{ odd}} + \left|\frac{J_{11}}{J_{22}}\right|^{1/4} \sum_{n\text{ even}}\right] \left|\frac{T_1'^2-4}{T_n'^2-4}\right|^{1/4} e^{i(nS_1/\hbar-\mu_n\pi/2)}, \qquad \theta_\text{f}\neq 0 \tag{3.5a}$$

where μ_n is given by Eq. (3.4a). For the orbit with $\theta_\text{f}=0$, we have

$$\psi^{\text{ret}}(\mathbf{q}) = \psi^{\text{out}}(\mathbf{q}_0) \left|\frac{\partial\theta_\text{f}}{\partial\theta_\text{i}}\right|^{-1} \sum_{n=1}^{\infty} \left|\frac{T_1^2-4}{T_n^2-4}\right|^{1/2} e^{i(nS_1/\hbar-\mu_n\pi/2)}, \qquad \theta_\text{f}=0 \tag{3.5b}$$

where μ_n is given by Eq. (3.4b).

4. EXAMPLES

We illustrate the uses of the above formulas by applying them to the "diamagnetic Kepler" problem, for which the Hamiltonian is

$$H=\tfrac{1}{2}(p_u^2+p_v^2)-4\varepsilon(u^2+v^2)+8u^2v^2(u^2+v^2)=2$$

[see Eq. (3.1)]. Two of the important periodic orbits in this system are: (i) "the perpendicular orbit," which lies on the ρ axis, or on the 45° line in the (u, v) plane, and therefore is type (1b) in Fig. 1; (ii) "the exotic X_1," which is a stable/unstable pair. These are shown in Fig. 2.

4.1. The Perpendicular Orbit

For this orbit we show in Fig. 3 the trace of the matrix $\mathbf{J}$ and the element $J_{12}=\partial v_1/\partial p_{v0}$ as function of ε. Both matrices are evaluated at the first return of the orbit (not at the period). Since the orbit is type 1,

$$J_{11}=J_{22}=\tfrac{1}{2}\operatorname{Tr}\mathbf{J}=\begin{cases}\cos\alpha_1=\cos\alpha_1' & \text{when stable}\\ \cosh\beta_1 & \text{when unstable}\end{cases}$$

The orbit is stable for $\varepsilon \leqslant -0.127...$ and unstable for larger ε. Figure 4 shows α_1 and β_1 as functions of ε. In this case the angles α_1, α_1', and $\tilde{\alpha}_1$ (defined in Appendix E) are all equal. [According to Apendix L, for this orbit Eq. (F6) gives the relationship between $\mathbf{K}$ and $\mathbf{J}$; clearly $\operatorname{Tr}\mathbf{K}=\operatorname{Tr}\mathbf{J}$

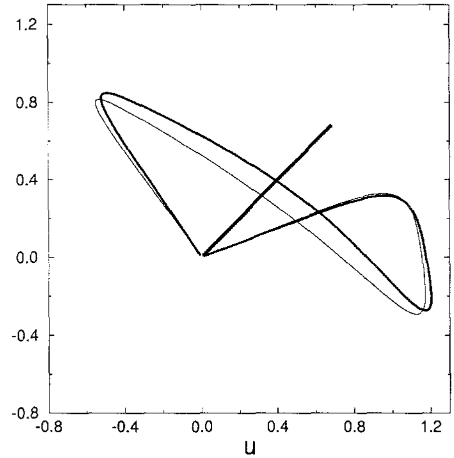

Fig. 2. Some orbits in the diamagnetic Kepler problem. In (u, v) coordinates the "perpendicular" orbit is a straight line at 45°. The "exotic X_1" is a pair of orbits, one stable and one unstable. All three orbits continue through the origin, and possess inversion symmetry in (u, v) space.

and since $\text{sgn}\, J_{12} = \text{sgn}\, K_{12} > 0$, $\tilde{\alpha}_1$ lies between 0 and π, and it is the same as α_1.]

Figure 5 shows the behavior of the classical amplitude A_n as a function of n for two values of ε. These graphs combine the results in Eqs. (2.1), (2.2), and (2.3c). At the higher value of ε, the orbit is unstable, and

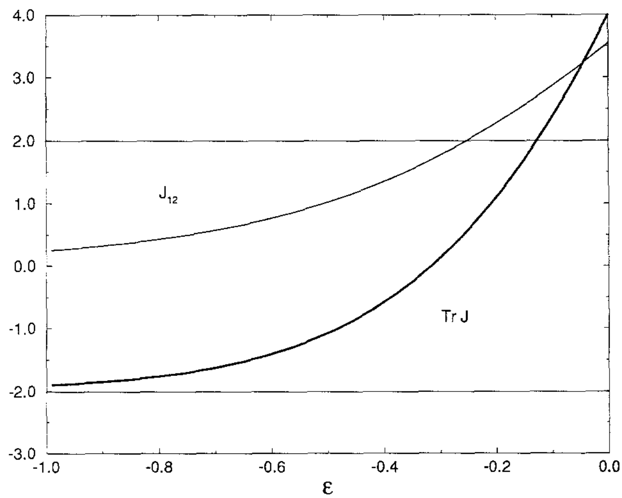

Fig. 3. The trace of the matrix **J** and the element J_{12} as functions of the parameter ε for the perpendicular orbit.

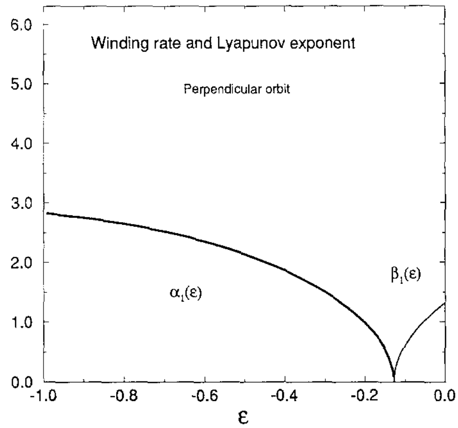

Fig. 4. The winding rate $\alpha_1(\varepsilon)$ and the Liapunov exponent $\beta_1(\varepsilon)$ for the perpendicular orbit.

A_n decreases approximately exponentially with n [more precisely, like $1/\sinh(n\beta_1)$]. At the lower value of ε, the orbit is stable, and A_n is proportional to $1/\sin(n\alpha_1)$. We see quasiperiodic behavior of A vs. n (it is a periodic function of n evaluated at discrete points having spacing unrelated to the period).

Table I shows the full Maslov index as a function of n for various

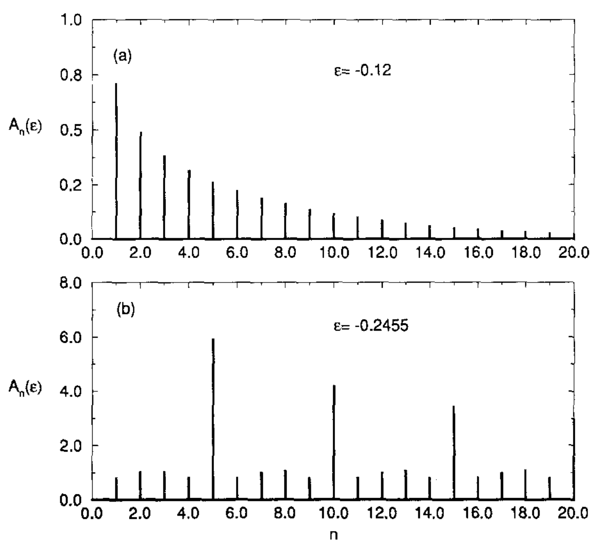

Fig. 5. The classical amplitude A_n vs. n for the perpendicular orbit at two values of ε. (a) The perpendicular orbit is unstable, and A_n decreases exponentially. (b) The orbit is stable and A_n oscillates quasiperiodically.

Table I. Maslov Indices at Various Scaled Energies for the Perpendicular Orbit[a]

	Return					
Energy	(1)	(2)	(3)	(4)	(5)	(6)
0.00	1	4	7	10	13	16
−0.14	1	4	7	10	13	16
−0.15	1	4	7	10	13	17
−0.16	1	4	7	10	14	17
−0.18	1	4	7	11	14	17
−0.21	1	4	8	11	14	18
−0.25	1	4	8	11	15	18
−0.32	1	5	8	12	15	19
−0.41	1	5	8	12	16	19
−0.49	1	5	9	12	16	20

[a] Points where the index changes are marked.

values of ε. For this orbit, as was shown in Fig. 4, the winding angle $\alpha_1 = \alpha_1' = \tilde{\alpha}_1$ is less than π for all ε. The phase point $(p_\sigma(t), \sigma(t))$ defined in Appendix E has moved less than a half cycle, so the Maslov index associated with crossing of the $\sigma = 0$ axis is zero. However (Appendix L) the orbit has an endpoint, so $\mu_1 = 1$ for all ε.

For $\varepsilon \leqslant -0.316...$, α_1 is greater than $\pi/2$. Since $J_{12} > 0$ (Fig. 3), we use the first of Eqs. (2.4b), and we find that on the second return the increment ν_2 to the Maslov index equals 1. For $\varepsilon \geqslant -0.316...$, α_1 is less than $\pi/2$, and this increment ν_2 equals 0. The two endpoints are counted by $n\mu_1$, and then we add 2 for the passage through the origin, for a total $\mu_2 = 4$ or 5. All of this is contained in Eq. (3.4a).

Values of $\mu_n(\varepsilon)$ for higher repetitions are understood in the same way.

4.2. The Exotic X_1

This is an orbit of type 2, discussed in Appendices I–K.

Each exotic is actually a member of a stable–unstable pair that is created in a saddle-center bifurcation. The two orbits have almost the same shape (in fact, the two are identical at their point of creation). At first closure, the full Maslov index of the stable one is 6, while that for the unstable one is 7. This includes 3 for crossings of axes, and either 3 or 4 for zeros of $\sigma(t)$. (Appendix E).

(It is easy to see geometrically why these two numbers must differ by 1. In Fig. 2, draw a neighbor of the two exotics that starts between them. Generally it will stay between them, since it must follow both orbits closely, but in general it will not close at the origin. Therefore it must cross one member of the pair once more than it crosses the other.)

We show in Fig. 6 various matrix elements of **J** for the stable and unstable X_1 as functions of ε near their point of creation. The trace is evaluated at a period (the second closure). It is equal to 2 at the creation point, and for higher ε it is greater than 2 for the unstable orbit, less than 2 for the stable one. The product $J_{11}J_{22}$ is evaluated at the first closure; the stable and unstable orbits have this product respectively less than or greater than 1. The matrix element J_{12} is negative for the stable orbit and positive for the unstable orbit.

For the unstable orbit, by calculation we find that all matrix elements of **J** are positive. Therefore the third line of Eq. (2.10) applies: $\nu_n = 0$, and (including passages through the origin) $\mu_n = 7n + 2(n-1) = 7, 16, 25, 34,\ldots$.

The stable exotic X_1 has interesting behavior that illustrates another of the formulas. It turns out that this initially stable orbit goes unstable above $\varepsilon \approx -0.115427$ via a period-doubling bifurcation. We have computed the

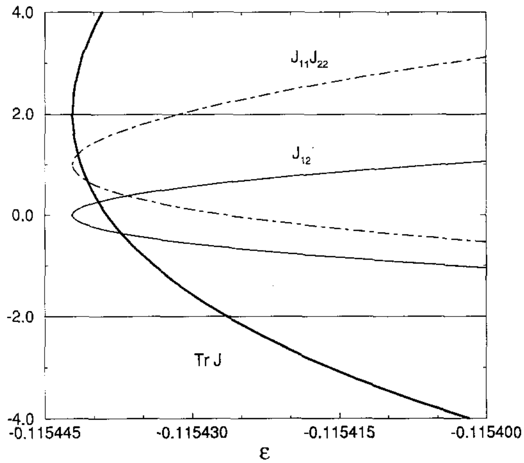

Fig. 6. Some matrix quantities for the exotic X_1 orbits. For every curve the upper branch is the unstable X_1 and the lower branch is the stable X_1. The heavy line is the trace of **J** evaluated at a period (second closure). For the unstable orbit it is greater than 2, and for the stable one it is less than 2. The broken line is the product $J_{11}J_{22}$ evaluated on the first closure. It is greater than 1 for the unstable orbit, and less than 1 for the stable one. The stable orbit goes unstable by a period-doubling bifurcation at $\varepsilon \approx -0.11527$ where $J_{11}J_{22}$ passes through 0 and the trace passes through -2. The finer solid line is J_{12}, which goes into the denominator of $A_1(\varepsilon)$.

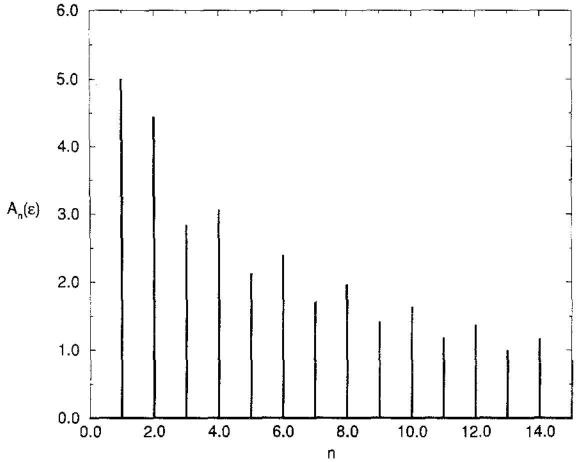

Fig. 7. Classical amplitude A_n vs. n for the unstable exotic. We see an alternation of intensity superimposed on an overall exponential decrease. The stable orbit has alternation of intensity superimposed on quasiperiodicity.

matrix **J** for this orbit at $\varepsilon = -0.11540$, and we find $J_{11} < 0$, $J_{12} < 0$, $J_{21} > 0$, $J_{22} > 0$. It follows that the last line in Eq. (2.10) is the relevant one, $v_n = \text{Int}(n/2)$, so $\mu_n = 6, 15, 23, 32, \ldots$.

The classical amplitude A_n follows the pattern described by Eq. (2.8). Superimposed on an overall exponential decrease there is an alternation of intensity between even and odd returns. This is shown for the initially unstable X_1 at $\varepsilon = -0.1154$ in Fig. 7.

In future work we will show how these amplitudes and Maslov indices manifest themselves in experimental observations of absorption spectra.

APPENDIX A. PROOF OF EQ. (2.1)

For a two-dimensional Hamiltonian system in polar $R\Theta$ space, the amplitude of the semiclassical wavefunction is given by

$$A_n = \left| \frac{J_{sc}(0, \Theta_i)}{J_{sc}(t_f, \Theta_i)} \right|^{1/2} \tag{A1}$$

where

$$J_{sc}(t, \Theta_i) = R \begin{vmatrix} \dfrac{\partial R}{\partial t} & \dfrac{\partial \Theta}{\partial t} \\ \dfrac{\partial R}{\partial \Theta_i} & \dfrac{\partial \Theta}{\partial \Theta_i} \end{vmatrix} \tag{A2}$$

and t_f is the time needed for traveling from the point (R_0, Θ_i) to (R_0, Θ_f) along the closed orbit. For any orbit closed at the origin in a two-dimensional Hamiltonian system with a smooth potential energy (no singularity or discontinuity at the origin, so $\partial V/\partial\Theta \to 0$ as $R \to 0$),

$$\left[\frac{\partial\Theta}{\partial t}\right]_{t=0} = \left[\frac{\partial\Theta}{\partial t}\right]_{t=t_f} \to 0, \qquad \text{as} \quad R_0 \to 0 \tag{A3}$$

Equation (A3) means that the trajectory is a straight line through the origin when it starts and returns to the origin. Therefore

$$\begin{aligned} J_{sc}(0, \Theta_i) &= \left.\frac{\partial R}{\partial t}\right|_{t=0} \equiv \dot{R}_i \\ J_{sc}(t_f, \Theta_i) &= \dot{R}_f \frac{\partial\Theta_f}{\partial\Theta_i} \end{aligned} \tag{A4}$$

and

$$A_n = \left(\frac{\dot{R}_i}{\dot{R}_f}\right)^{1/2} \left|\frac{\partial\Theta_f}{\partial\Theta_i}\right|^{-1/2} \tag{A5}$$

The initial and final speeds are equal if the Hamiltonian has the usual form (i.e., kinetic energy plus potential energy), if $V(0, \Theta_i) = V(0, \Theta_f)$, and if Eq. (A3) holds. The latter two hold for any potential energy that is smooth near the origin, and also for systems with attractive Coulomb singularities. Under this condition, Eq. (A5) becomes Eq. (2.1) in the text.

APPENDIX B. PROOF OF EQ. (2.2)

See Fig. 8 and the caption. The circle is assumed to be sufficiently small that inside the circle the outgoing orbits are straight radial lines and returning orbits are straight parallel lines. Since the system is conservative (i.e., $E = \text{const}$) and the orbit is closed at the origin (i.e., $u_0 = v_0 = 0$ are the initial coordinates), we may regard u and v as functions of only the v component of the initial momentum and time,

$$\begin{aligned} u &= u(p_{vi}, t) \\ v &= v(p_{vi}, t) \end{aligned} \tag{B1}$$

where

$$p_{vi} = m\dot{R}_i \sin\Theta_i \tag{B2}$$

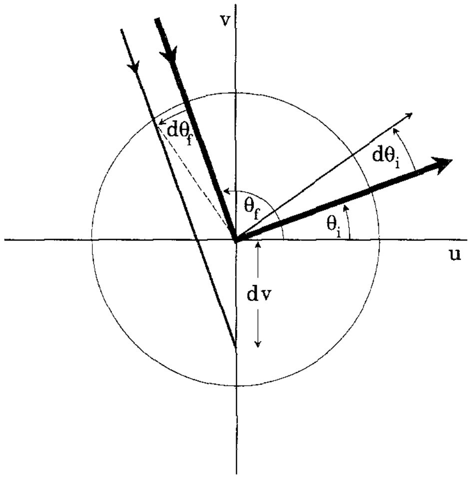

Fig. 8. (u, v) are a "right-oriented" coordinate system, and angles θ are measured from the u axis with counterclockwise being positive. A closed orbit leaves at initial angle Θ_i and returns at final angle Θ_f. Its initial v component of momentum is p_{vi}. The neighbor of the closed orbit leaves, also moving radially outward, at angle $\Theta_i + d\Theta_i$, so its initial momentum component is $p_{vi} + dp_{vi}$; $dp_{vi}/d\Theta_i = |\mathbf{p}_i| \cos \Theta_i$. The neighbor returns to the boundary circle R_0 at angle $\Theta_f + d\Theta_f$. It continues on a straight line, and passes through the $u=0$ axis at the point dv_f. Equation (2.2) relates $(\partial v_f/\partial p_{vi})_{u=0}$ to $(\partial \Theta_f/\partial \Theta_i)_{R=R_0}$.

Therefore

$$J_{12} \equiv \left(\frac{\partial v}{\partial p_{vi}}\right)_{u=0} = \left(\frac{\partial v}{\partial p_{vi}}\right)_t + \left(\frac{\partial v}{\partial t}\right)_{p_{vi}} \left(\frac{\partial t}{\partial p_{vi}}\right)_{u=0} \tag{B3}$$

The last derivative in the equation above is given by

$$du = 0 = \left(\frac{\partial u}{\partial t}\right)_{p_{vi}} dt + \left(\frac{\partial u}{\partial p_{vi}}\right)_t dp_{vi}$$

Hence

$$J_{12} = \left(\frac{\partial v}{\partial p_{vi}}\right)_t - \left(\frac{\partial u}{\partial p_{vi}}\right)_t \frac{(\partial v/\partial t)_{p_{vi}}}{(\partial u/\partial t)_{p_{vi}}} \tag{B4}$$

The ratio $\dot{v}_f/\dot{u}_f$ in Eq. (B4) is $\tan \Theta_f$ because the orbit is closed at the origin. Using Eq. (B2), we have

$$J_{12} = \frac{1}{m\dot{R}_i \cos \Theta_i \cos \Theta_f} \left[\left(\frac{\partial v}{\partial \Theta_i}\right)_t \cos \Theta_f - \left(\frac{\partial u}{\partial \Theta_i}\right)_t \sin \Theta_f\right] \tag{B5}$$

The derivatives $(\partial v/\partial \Theta_i)_t$ and $(\partial u/\partial \Theta_i)_t$ can be evaluated on the returning circle, where $u = R_0 \cos \Theta_f$ and $v = R_0 \sin \Theta_f$, and $\partial u/\partial \Theta_i = -R_0 \sin \Theta_f (\partial \Theta_f/\partial \Theta_i)$, etc. Therefore

$$J_{12} = \frac{R_0}{m\dot{R}_i \cos \Theta_i \cos \Theta_f} \frac{\partial \Theta_f}{\partial \Theta_i} \tag{B6}$$

For the nth return of the closed orbit, denote Θ_f as $\Theta_f(n)$, and arrive at Eq. (2.2).

APPENDIX C. SELF-MULTIPLICATION OF A 2×2 MATRIX WITH DETERMINANT EQUAL TO 1

Let **J** be a 2×2 matrix with Det **J** = 1, so its eigenvalues are λ and λ^{-1} ($|\lambda| \geqslant 1$), and let **U** be an invertible transformation which diagonalizes **J**,

$$\mathbf{j} = \mathbf{U}^{-1}\mathbf{J}\mathbf{U} = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda^{-1} \end{bmatrix} \tag{C1}$$

Assume det $U = 1$ (or multiply U by a constant to make det $U = 1$). The nth self-multiplication of **J** is then

$$\mathbf{J}^n = \mathbf{U}\mathbf{j}^n\mathbf{U}^{-1} = \begin{bmatrix} \lambda^n u_{11}u_{22} - \lambda^{-n}u_{12}u_{21} & (-\lambda^n + \lambda^{-n})u_{11}u_{12} \\ (\lambda^n - \lambda^{-n})u_{21}u_{22} & -\lambda^n u_{12}u_{21} + \lambda^{-n}u_{11}u_{22} \end{bmatrix} \tag{C2}$$

where u_{11}, u_{12}, u_{21}, and u_{22} are the elements of **U**.

For $n = 1$, Eq. (C2) gives

$$\mathbf{J} = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} = \begin{bmatrix} \lambda u_{11}u_{22} - \lambda^{-1}u_{12}u_{21} & (-\lambda + \lambda^{-1})u_{11}u_{12} \\ (\lambda - \lambda^{-1})u_{21}u_{22} & -\lambda u_{12}u_{21} + \lambda^{-1}u_{11}u_{22} \end{bmatrix} \tag{C3}$$

Let us regard this as four equations for products of elements of U. Solving these equations, we have

$$\begin{aligned} u_{11}u_{12} &= -\frac{J_{12}}{\lambda - \lambda^{-1}}, & u_{11}u_{22} &= \frac{J_{11} - \lambda^{-1}}{\lambda - \lambda^{-1}} \\ u_{21}u_{22} &= \frac{J_{21}}{\lambda - \lambda^{-1}}, & u_{12}u_{21} &= \frac{J_{11} - \lambda}{\lambda - \lambda^{-1}} \end{aligned} \tag{C4}$$

Substituting Eq. (C4) into Eq. (C2), we have

$$\mathbf{J}^n = D'_{n-1}\mathbf{J} - D'_{n-2} \tag{C5}$$

where D'_m is defined by

$$D'_m \equiv \frac{\lambda^{m+1} - \lambda^{-(m+1)}}{\lambda - \lambda^{-1}} \tag{C6}$$

From this definition, the recursion relation of D'_m is

$$D'_m = T_1 D'_{m-1} - D'_{m-2} \tag{C7}$$

where $T_1 = \lambda + \lambda^{-1}$ is the trace of $\mathbf{J}$.

For stable orbits, $\lambda = \exp(\pm i\alpha_1)$. For unstable orbits, $\lambda = (\operatorname{sgn} T_1) \exp(\pm\beta_1)$. Therefore, according to Eq. (C6),

$$|D'_{n-1}| = \begin{cases} \dfrac{\sin(n\alpha_1)}{\sin\alpha_1}, & \text{stable} \\ \dfrac{\sinh(n\beta_1)}{\sinh\beta_1}, & \text{unstable} \end{cases} \tag{C8}$$

It is easy to show that $|D'_{n-1}|$ can be expressed in terms of the trace of the stability matrices as

$$|D'_{n-1}| = \left|\frac{T_n^2 - 4}{T_1^2 - 4}\right|^{1/2} \tag{C9}$$

where T_n is the trace of $\mathbf{J}^n$.

From Eq. (C5) we have

$$[\mathbf{J}^n]_{12} = J_{12} D'_{n-1} \tag{C10}$$

This is Eq. (2.3) in the text.

In the special case that $J_{11} = J_{22}$, D'_m is the Chebyshev polynomial of the second kind, denoted $D_m(J_{11})$. This is because the recursion relation of D'_m is, according to Eq. (C7),

$$D'_m(J_{11}) = 2J_{11} D'_{m-1}(J_{11}) - D'_{m-2}(J_{11}) \tag{C11}$$

which is the same as the recursion relation of the Chebyshev polynomials, and because $D'_1 = 1 = D_1(J_{11})$ and $D'_2 = 2J_{11} = D_2(J_{11})$ according to the definition of D'_m in Eq. (C6). Therefore Eq. (C5) can be written as

$$\mathbf{J}^n = \begin{bmatrix} C_n(J_{11}) & J_{12} D_{n-1}(J_{11}) \\ J_{21} D_{n-1}(J_{11}) & C_n(J_{11}) \end{bmatrix} \tag{C12}$$

where $C_m(J_{11})$ and $D_m(J_{11})$ are Chebyshev polynomials of the first and the second kinds. Here we have used the relation between C_m and D_m,

$$C_m(x) = D_m(x) - x D_{m-1}(x) \tag{C13}$$

and the recursion relations for C_m and D_m,

$$\begin{aligned} C_m(x) &= 2xC_{m-1}(x) - C_{m-2}(x) \\ D_m(x) &= 2xD_{m-1}(x) - D_{m-2}(x) \end{aligned} \tag{C14}$$

We define α_1 such that

$$\cos\alpha_1 = \begin{cases} J_{11}, & \text{if } |J_{11}| < 1 \\ s'J_{11}, \quad s' \equiv \operatorname{sgn}(J_{11} + J_{22}), & \text{if } |J_{11}| > 1 \end{cases} \tag{C15}$$

where α_1 is real $(0 < \alpha_1 < \pi)$ if $|J_{11}| < 1$ (stable), and $\alpha_1 = i\beta_1$, where β_1 is the (positive) Lyapunov exponent, if $|J_{11}| > 1$ (unstable). Using the properties of the Chebyshev polynomials,

$$\begin{aligned} C_m(\cos\alpha) &= \cos(m\alpha) \\ D_m(\cos\alpha) &= \frac{\sin(m+1)\alpha}{\sin\alpha} \end{aligned} \tag{C16}$$

and

$$\begin{aligned} C_m(\pm x) &= (\pm)^m\, C_m(x) \\ D_m(\pm x) &= (\pm)^m\, D_m(x) \end{aligned} \tag{C17}$$

we obtain for Eq. (C12)

$$\mathbf{J}^n = \begin{bmatrix} \cos(n\alpha_1) & J_{12}\dfrac{\sin(n\alpha_1)}{\sin\alpha_1} \\ J_{21}\dfrac{\sin(n\alpha_1)}{\sin\alpha_1} & \cos(n\alpha_1) \end{bmatrix}, \quad \text{stable} \tag{C18a}$$

$$\mathbf{J}^n = (s')^{n-1} \begin{bmatrix} s'\cos(n\alpha_1) & J_{12}\dfrac{\sin(n\alpha_1)}{\sin\alpha_1} \\ J_{21}\dfrac{\sin(n\alpha_1)}{\sin\alpha_1} & s'\cos(n\alpha_1) \end{bmatrix}, \quad \text{unstable} \tag{C18b}$$

APPENDIX D. LINEARIZATION ABOUT A PERIODIC ORBIT

For a system with two degrees of freedom, equations of motion for small displacement about a periodic orbit are derived. Our approach is slightly different from that used by others.[4] Most authors set up a set of four linear equations, and an associated 4×4 monodromy matrix, then they discard irrelevant information in this matrix, reducing it to 2×2. We reduce the system to two linear differential equations first; then the associated Jacobian matrix is already in the desired form.

We assume that the periodic orbit has no endpoints, i.e., no point at which the speed vanishes and the orbit turns around to retrace itself. Most of our conclusions still hold even for such orbits, but the proofs require additional discussion, given in Appendix L.

D1. Locally Cartesian Coordinates near a Periodic Orbit

Given a coordinate system (u, v) with orthogonal unit vectors $(\hat{\imath}, \hat{\jmath})$ along the axes, and given a periodic orbit $\{u(t), v(t) \mid 0 \leqslant t < T\}$, we define $\Lambda(t)$ to be the arc length along the orbit, such that $\Lambda(t=0)=0$ and

$$d\Lambda(t)/dt = [(du(t)/dt)^2 + (dv(t)/dt)^2]^{1/2}$$

At each point on the orbit, define a unit vector $\hat{\lambda}(t)$ along the orbit in the direction of motion, and a second vector $\hat{\sigma}(t)$ perpendicular to it and pointing to the left (Fig. 9),

$$\begin{aligned}\hat{\lambda}(t) &= \left[\hat{\imath}\frac{du}{dt} + \hat{\jmath}\frac{dv}{dt}\right] \Big/ \left[\left(\frac{du}{dt}\right)^2 + \left(\frac{dv}{dt}\right)^2\right]^{1/2} \\ \hat{\sigma}(t) &= \left[-\hat{\imath}\frac{dv}{dt} + \hat{\jmath}\frac{du}{dt}\right] \Big/ \left[\left(\frac{du}{dt}\right)^2 + \left(\frac{dv}{dt}\right)^2\right]^{1/2}\end{aligned} \tag{D1}$$

It is convenient also to define the angle $\phi(t)$ between $\hat{\lambda}(t)$ and the u axis,

$$\cos\phi(t) = \hat{\lambda}(t)\cdot\hat{\imath}, \qquad \sin\phi(t) = \hat{\lambda}(t)\cdot\hat{\jmath} \tag{D2}$$

For every sufficiently small range of time $(t_1 < t < t_2)$, these two unit vectors provide a coordinate grid which spans a strip around the periodic orbit. Specifically, for every (u, v) in a sufficiently small strip, drop a straight line to the nearest point on the periodic orbit, and specify coordinates of that point (λ, σ) such that (i) $|\sigma|$ is the distance to the orbit, and σ is positive on the left and negative on the right; (ii) λ is $\Lambda(t)$ at the point that the straight line intersects the orbit.

[4] See, e.g., Gutzwiller[(7)] and Poincaré.[(8)] Our method takes an idea from de Aguiar *et al.*[(9)]

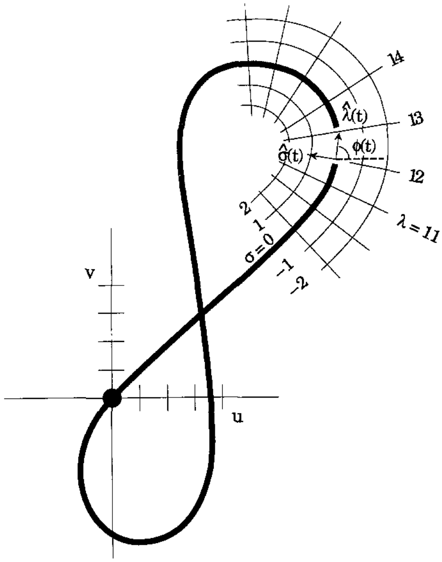

Fig. 9. Locally Cartesian coordinates about a periodic orbit. Coordinates (λ, σ) are also "right-oriented" to make $\partial(u, v)/\partial(\lambda, \sigma) \approx 1$. Here $\hat{\lambda}$ is along tyhe orbit and $\hat{\sigma}$ is across it. The angle between coordinates (u, v) and (λ, σ) is $\phi(t)$.

With those definitions, one can verify that the Jacobian matrix connecting these coordinate systems is

$$\begin{bmatrix} \dfrac{\partial u}{\partial \lambda} & \dfrac{\partial u}{\partial \sigma} \\ \dfrac{\partial v}{\partial \lambda} & \dfrac{\partial v}{\partial \sigma} \end{bmatrix} = \begin{bmatrix} a(\lambda, \sigma)\cos\phi & -\sin\phi \\ a(\lambda, \sigma)\sin\phi & \cos\phi \end{bmatrix} \tag{D3}$$

where

$$a(\lambda, \sigma) \equiv 1 - \sigma/r_0(\lambda) \tag{D4}$$

$$r_0(\lambda) = \left(\frac{d\phi}{\partial\lambda}\right)^{-1} = \left(\frac{d\phi(t)/dt}{dA(t)/dt}\right)^{-1} \tag{D5}$$

$r_0(\lambda)$ can be positive or negative; its magnitude $|r_0(\lambda)|$ is the instantaneous radius of curvature of the periodic orbit, while $|r_0(\lambda) - \sigma|$ is the radius of curvature of the curve of constant σ at that same value of λ. The function $r_0(\lambda)$ is positive whenever the periodic orbit is curving to the left as we face along the orbit. The Jacobian determinant equals unity for $\sigma = 0$, and it is nonvanishing in a strip around the periodic orbit.

D2. Canonical Transformation to ($\lambda\sigma p_\lambda p_\sigma$) Coordinates

Using a type 3 generating function,

$$W_3(p_u, p_v; \lambda, \sigma) = -p_u u(\lambda, \sigma) - p_v v(\lambda, \sigma) \tag{D6}$$

we find

$$\begin{aligned} p_\lambda &= p_u \frac{\partial u}{\partial \lambda} + p_v \frac{\partial v}{\partial \lambda} = a(\lambda, \sigma)[p_u \cos\phi + p_v \sin\phi] \\ p_\sigma &= p_u \frac{\partial u}{\partial \sigma} + p_v \frac{\partial v}{\partial \sigma} = -p_u \sin\phi + p_v \cos\phi \end{aligned} \tag{D7}$$

so the Hamiltonian is

$$H = (1/2m)[p_\lambda^2/a(\lambda, \sigma)^2 + p_\sigma^2] + V(\lambda, \sigma) \tag{D8}$$

with the potential energy now reexpressed as a function of λ and σ.

On the periodic orbit $\sigma(t) = 0$, $\dot{\sigma}(t) = p_\sigma(t)/m = 0$, and we write $\lambda(t) = \Lambda(t)$ (as before) and $p_\lambda(t) = P_\Lambda(t)$. Also, on the periodic orbit, since $dp_\sigma/dt = -\partial H/\partial\sigma = 0$,

$$\frac{P_\Lambda^2}{mr_0} + \frac{\partial V}{\partial \sigma} = 0 \tag{D9}$$

(i.e., $m\dot{\Lambda}^2/r_0 = -\partial V/\partial\sigma$; the centripetal acceleration is proportional to the centripetal force).

D3. Small Displacements from the Periodic Orbit

Consistent with the assumption that the orbit has no endpoints, we assume that on the periodic orbit $\dot{\Lambda}(t)$ never vanishes, and that it is bounded away from zero $\dot{\Lambda}(t) \geqslant \varepsilon > 0$. Then for all points in phase space sufficiently close to the periodic orbit, $d\lambda/dt$ will also be positive. We can then use λ as the independent variable instead of t, and set up equations of motion for $d\sigma/d\lambda \equiv (d\sigma/dt)/(d\lambda/dt)$.

The resulting equations of motion have Hamiltonian form; i.e., there exists a function $K(p_\sigma, \sigma; \lambda)$ such that

$$\frac{d\sigma}{d\lambda} = \frac{\partial K}{\partial p_\sigma}, \qquad \frac{dp_\sigma}{d\lambda} = -\frac{\partial K}{\partial \sigma} \tag{D10}$$

For trajectories of specified energy E, that effective Hamiltonian is obtained by solving the equation $H(p_\lambda, p_\sigma, \lambda, \sigma) = E$ to obtain the function $p_\lambda(p_\sigma, \sigma; \lambda; E)$. The effective Hamiltonian is (minus) that function:

$$K(p_\sigma, \sigma; \lambda) = -p_\lambda(p_\sigma, \sigma; \lambda; E) \tag{D11a}$$

$$= -\left\{2m\left[1 - \frac{\sigma}{r_0(\lambda)}\right]^2 \left[E - \frac{p_\sigma^2}{2m} - V(\lambda, \sigma)\right]\right\}^{1/2} \tag{D11b}$$

Proof of Eq. (D11a):

$$\frac{d\sigma}{d\lambda} = \frac{d\sigma/dt}{d\lambda/dt} = \frac{\partial H/\partial p_\sigma}{\partial H/\partial p_\lambda} = -\left(\frac{\partial p_\lambda}{\partial p_\sigma}\right)_{\lambda, \sigma, E}$$

and similarly for $dp_\sigma/d\lambda$.

The general equations of motion are complicated, but we do not need them, We only note that in lowest order, the linearized equations of motion are

$$\frac{d\sigma}{d\lambda} = \frac{p_\sigma}{P_\Lambda(\lambda)}$$
$$\frac{dp_\sigma}{d\lambda} = -\frac{m}{P_\Lambda(\lambda)}\left[\left.\frac{\partial^2 V(\lambda, \sigma)}{\partial \sigma^2}\right|_{\sigma=0} + \frac{3P_\Lambda^2(\lambda)}{mr_0^2(\lambda)}\right]\sigma \tag{D12a}$$

or, switching back to an effective-time variable τ, with $d\lambda/d\tau = P_\Lambda(\lambda)/m$,

$$\frac{d\sigma}{d\tau} = \frac{p_\sigma}{m}$$
$$\frac{dp_\sigma}{d\tau} = -\left[\frac{\partial^2 V(\tau)}{\partial \sigma^2} + \frac{3P_\Lambda^2(\tau)}{mr_0^2(\tau)}\right]\sigma \tag{D12b}$$

These are the equations of motion of a harmonic oscillator with a periodic force constant, i.e., they are Hill's equation.

For much of what follows, we only need to know that the effective Hamiltonian $K(p_\sigma, \sigma; \lambda)$ exists. Equations (D10) imply that the evolution in λ is the continuous unfolding or development of a canonical transformation. Therefore the motion in the (p_σ, σ) plane is described by a continuous group of canonical mappings. If we integrate through one cycle of the periodic orbit, stopping when $\lambda = \Lambda(T)$, then we have a Poincaré map associated with the orbit. This Poincaré map is a member of the continuous family of canonical maps which describe the evolution of the phase point $(p_\sigma(\tau), \sigma(\tau))$.

In principle t and τ are not the same. They are related by

$$\frac{d\tau}{dt}=\frac{d\tau/d\lambda}{dt/d\lambda}=\frac{p_\lambda(p_\sigma,\sigma;\lambda;E)}{P_A(\lambda)}=1+O(p_\sigma^2,\sigma^2)$$

However, they are the same to first order in p_σ and σ, and we have no further need to distinguish between them. In the following we go back to writing t as the independent variable, but we remember that the Poincaré map is in principle defined by stopping at fixed λ ($\equiv$fixed τ).

APPENDIX E. WINDING NUMBER AND MASLOV INDEX

We define a "winding angle" $\tilde{\alpha}(t)$ such that for any point $A(t)$ on the periodic orbit, the Maslov index is

$$\mu=\mathrm{Int}[\tilde{\alpha}(t)/\pi] \tag{E1}$$

where $\mathrm{Int}(z)$ is the largest integer less than z.

Let us recall that a Maslov index is not a property of a periodic orbit by itself. Formally it is defined as a property of a curve on a Lagrangian manifold; i.e., it is a property of an orbit within a family of orbits. For the Green functions considered in this paper, the orbits all begin radially outward from the origin with a fixed total energy. Thus, surrounding the periodic orbit, having initial conditions ($\lambda=0$, $\sigma=0$, $p_\lambda=P_A(0)$, $p_\sigma=0$), we consider the family of orbits having $\lambda=0$, $\sigma=0$, p_σ small but arbitrary, $p_\lambda=P_A(0)-O(p_\sigma^2)$. The behavior of $\sigma(t)$ and $p_\sigma(t)$ can be determined by integrating Hill's equation,

$$\dot{\sigma}=p_\sigma/m \tag{E2a}$$

$$\dot{p}_\sigma=-k_\sigma(t)\sigma \tag{E2b}$$

where $k_\sigma(t)$ is periodic.

In Fig. 10 we show qualitatively a typical solution to Hill's equation plotted in the (σ, p_σ) phase plane. One important property follows trivially from Eq. (E2a): the phase point only passes through the positive p_σ axis moving right, and through the negative p_σ axis moving left. The motion up and down in the phase plane can be quite complicated, but the sideways motion is simple: it is to the right in the upper half-plane and to the left in the lower half-plane.

As stated above, the initial conditions for all orbits are $\sigma=0$, p_σ small and arbitrary. Hence all orbits start on the p_σ axis and begin moving in a clockwise sense. Because the equations are linear, the locus of phase points at any time t is a straight line. Let the angle between this straight line

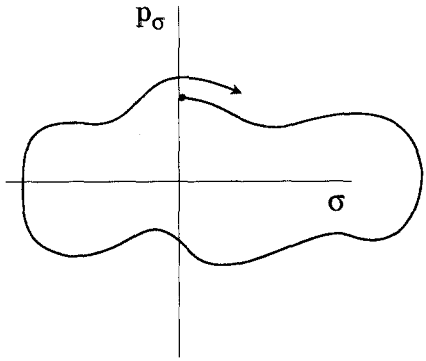

Fig. 10. Qualitative phase track. Phase track of a point that moves according to Hill's equation.

and the p_σ axis be denoted $\tilde{\alpha}(t)$. Equivalently, follow any one such phase point through time, starting on the positive p_σ axis, and define $\tilde{\alpha}(t) = \tan^{-1}[\sigma(t)/p_\sigma(t)]$. The function $\tilde{\alpha}(t)$ is not necessarily monotonic, but at least $d\tilde{\alpha}(t)/dt > 0$ whenever $k_\sigma(t) > 0$ and also $d\tilde{\alpha}(t)/dt > 0$ whenever $\sigma(t) = 0$.

Caustics arise whenever the projection from the Lagrangian manifold to configuration space is singular, i.e., whenever the Jacobian $J_{\text{sc}} = \partial(u, v)/\partial(t, p_\sigma^0)$ vanishes. Transforming coordinates from (u, v) to (λ, σ), we obtain

$$J_{\text{sc}} = \frac{\partial(u, v)}{\partial(t, p_\sigma^0)} = \frac{\partial(u, v)}{\partial(\lambda, \sigma)} \frac{\partial(\lambda, \sigma)}{\partial(t, p_\sigma^0)}$$

From Eq. (D3), the first factor does not vanish. For small displacements, the second factor approaches

$$\lim_{p_\sigma^0 \to 0} \frac{\partial(\lambda, \sigma)}{\partial(t, p_\sigma^0)} = \dot{\Lambda}(t) \frac{\partial\sigma(t, p_\sigma^0)}{\partial p_\sigma^0} = \dot{\Lambda}(t)\, \sigma(t)$$

The displacement $\sigma(t, p_\sigma^0)$ is linearly proportional to the initial momentum p_σ^0, and we write $\sigma(t)$ as the displacement that is obtained for unit initial momentum, $\sigma(t) = \sigma(t, 1)$. Since by assumption we deal only with trajectories on which $\dot{\Lambda}(t)$ never vanishes, caustics occur when $\sigma(t)$ passes through zero. Furthermore, under this condition, only simple "fold-type" caustics can occur. As a result, the Maslov index changes by 1. Finally, it is known that for Hamiltonians of the usual $\mathbf{p}^2/2m + V(q)$ form, the Maslov index only increases with time as we move forward along the trajectory. (This is connected with the direction in which the phase point crosses the p_σ axis.)

It follows that the Maslov index at any point along the trajectories is equal to the number of crossings the phase point has made with the p_σ axis, i.e.,

$$\mu = \mathrm{Int}[\tilde{\alpha}(t)/\pi] \tag{E3}$$

By convention the Maslov index at the beginning of the orbit is zero. This means that we do not count the initial point as a crossing of the positive p_σ axis. In the following we will say that the initial phase point is just to the right of the positive p_σ axis.

A second way of expressing Eq. (E3) is especially convenient. The solutions $\{\sigma(t), p_\sigma(t)\}$ to Hill's equation (E2) are linear functions of the initial conditions, so there exists a matrix $K(t)$ such that

$$\begin{bmatrix} \sigma(t) \\ p_\sigma(t) \end{bmatrix} = \mathbf{K}(t) \begin{bmatrix} \sigma(0) \\ p_\sigma(0) \end{bmatrix} \tag{E4}$$

Initially the element $K_{12}(t)$ is 0^+ and $dK_{12}/dt > 0$. Equation (E3) is equivalent to the statement that the Maslov index at any point is equal to the number of times $K_{12}(t')$ has changed sign for $0 < t' < T$.

APPENDIX F. MASLOV INDEX AT A PERIOD

Now we "strobe" the motion in the (σ, p_σ) plane, observing the location of the phase point at each period T of the coefficient $k_\sigma(t)$. This defines a Poincaré map $(\sigma_n, p_{\sigma n})$ to $(\sigma_{n+1}, p_{\sigma n+1})$. The map is area-preserving and linear, and we denote it

$$\begin{pmatrix} \sigma_{n+1} \\ p_{\sigma_{n+1}} \end{pmatrix} = \mathbf{K}(T) \begin{pmatrix} \sigma_n \\ p_{\sigma_n} \end{pmatrix} \tag{F1}$$

$\mathbf{K}(T)$ is the matrix that represents the solutions to Hill's equation at a period.

As before, the initial conditions on the map are $\sigma = 0$, p_σ arbitrary but for convenience positive. Hence $\tilde{\alpha}_0 = 0$. The strobed transformation $K(T)$ at a period describes the change of $p_\sigma(t)$ and $\sigma(t)$ over a cycle of $k_\sigma(t)$, but omitting one important detail: it does not tell how many full revolutions of the phase point have occurred. If we only determine the matrix $\mathbf{K}(T)$ we have determined $\tilde{\alpha}(T)$ only modulo 2π. The number of full revolutions of the phase point which are hidden in $\mathbf{K}(T)$ is given by $\mathrm{Int}[\mu(T)/2] \equiv \mathrm{Int}(\mu_1/2)$.

Suppose the central orbit is stable. Then $|\mathrm{Tr}\,\mathbf{K}| < 2$. We show in Appendix G that there exists a canonical linear change of coordinates which converts the mapping into a pure rotation. In the new variables (σ'', p''_σ) the phase angle $\tilde{\alpha}'' = \tan^{-1}(\sigma''/p''_\sigma)$ increases by a fixed amount in each cycle,

$$\tilde{\alpha}''((n+1)T) - \tilde{\alpha}''(nT) = 2\pi \, \mathrm{Int}(\mu_1/2) + \tilde{\alpha}_1 \tag{F2}$$

The first term is the number of full revolutions, and the second is the additional partial revolution of the phase point occurring within a single cycle. $\tilde{\alpha}_1$ can be calculated from $\mathbf{K}$ using Eq. (G9).

The linear change of coordinates converts any straight line through the origin to another straight line through the origin. It follows that the number of complete half-cycles through which the phase point has advanced is invariant under this linear transformation,

$$\mathrm{Int}\left[\frac{\tilde{\alpha}(nT) - \tilde{\alpha}(0)}{\pi}\right] = \mathrm{Int}\left[\frac{\tilde{\alpha}''(nT) - \tilde{\alpha}''(0)}{\pi}\right] \tag{F3}$$

The left-hand side is the Maslov index for the nth return. If we combine this equation with (F2) and apply it to the first return, we find that if μ_1 is even,[5] then $\tilde{\alpha}_1$ must lie between 0 and π, so $K_{12}(T) > 0$, while if μ_1 is odd, then $\tilde{\alpha}_1$ must lie between π and 2π and $K_{12}(T) < 0$. Then finally applying these two equations to the nth return, we obtain

$$\mu_n = 2n \, \mathrm{Int}(\mu_1/2) + \mathrm{Int}(n\tilde{\alpha}_1/\pi) \tag{F4}$$

Now suppose the orbit is unstable, and $|\mathrm{Tr}\,\mathbf{K}| > 2$. In this case, a linear transformation converts the map into a hyperbolic rotation (with reflection if $\mathrm{Tr}\,\mathbf{K} < -2$). We must always remember that the initial phase point starts just to the right of the original p_σ axis, and that the continuous motion is in a generally clockwise sense. Strobing this motion at the map time leads to one of the sequences of points shown in Fig. 11.

Define $s_1 = \mathrm{sgn}(\mathrm{Tr}\,\mathbf{K})$, $s_2 = \mathrm{sgn}\, K_{12}$. Consider the case $s_1 s_2 > 0$ and $\mathrm{Tr}\,\mathbf{K} > 0$. Then successively strobed phase points march to the right on the upper hyperbola. It follows that μ_1 is even (see footnote 5) and $\mu_n = n\mu_1$. If $s_1 s_2 > 0$ and $\mathrm{Tr}\,\mathbf{K} < 0$, phase points alternate between the two branches of the hyperbola. It follows that μ_1 is odd and again $\mu_n = n\mu_1$.

Now consider the case $s_1 s_2 < 0$ and $\mathrm{Tr}\,\mathbf{K} > 0$. This time successive points march leftward on the upper hyperbola. Since the initial point was just to the right of the p_v axis, μ_1 must be odd. Also the change of μ on every cycle after the first must be $\mu_1 + 1$. Therefore $\mu_n = n\mu_1 + n - 1$.

[5] Everywhere that we refer to μ_1 being odd or even, we are referring to that part of μ_1 that comes from zeros of $\sigma(t)$ (excluding any additional contribuition from a z-axis crossing, Coulomb singularity, endpoint, etc.).

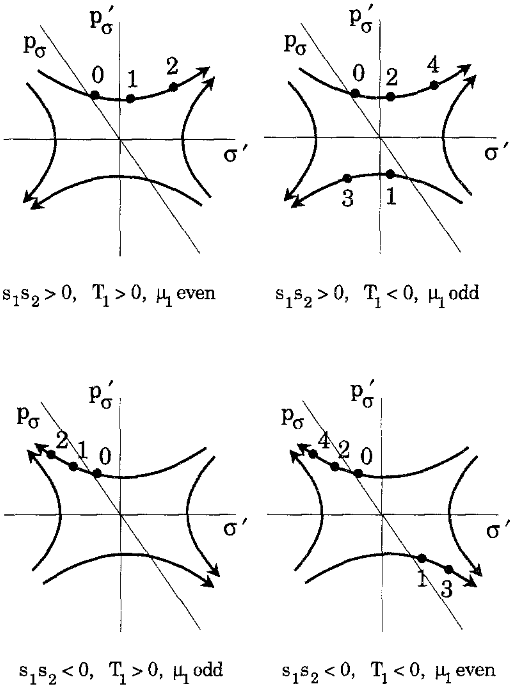

Fig. 11. Sequence of points in the (σ', p_σ') plane for unstable orbits. In the principal-axis frame, the motion is a hyperbolic rotation with or without reflection. If $s_1 s_2 > 0$, we have a "positive hyperbolic rotation." The phase point begins just to the right of the p_σ axis and moves continuously in a clockwise sense. At each period T, the phase point lands according to the indicated sequence. See also footnote 5.

Finally, if $s_1 s_2 < 0$ and $\operatorname{Tr} \mathbf{K} < 0$, by the same reasoning μ_1 is even and again $\mu_n = n\mu_1 + n - 1$. The above results can be summarized by the formula for the unstable case:

$$\begin{aligned} &s_1 s_2 = \operatorname{sgn}(K_{12} \operatorname{Tr} \mathbf{K}) \\ &\mu_n = n\mu_1 + \nu_n \\ &\nu_n = 0 \qquad \text{if} \quad s_1 s_2 > 0 \\ &\nu_n = n - 1 \qquad \text{if} \quad s_1 s_2 < 0 \end{aligned} \tag{F5}$$

We have almost succeeded in proving Eq. (2.4). However, note that the Jacobian matrix in this Appendix is the one associated with the (σ, p_σ) map, whereas the matrix discussed in the text is the one associated with the

(v, p_v) map. It is not hard to show that for periodic orbits these two matrices are related by

$$\mathbf{K}(nT)=\begin{bmatrix} J_{11}(n) & \cos^2\Theta_i\, J_{12}(n) \\ \dfrac{1}{\cos^2\Theta_i} J_{21}(n) & J_{22}(n) \end{bmatrix} \tag{F6}$$

It follows that $\mathrm{Tr}\,\mathbf{K}(T)=\mathrm{Tr}\,\mathbf{J}(1)$ and $\mathrm{sgn}\,K_{12}(T)=\mathrm{sgn}\,J_{12}(1)$. Therefore it is not necessary to solve Hill's equation or to calculate $\mathbf{K}(T)$—all the required information is contained in μ_1 and $\mathbf{J}(1)$. We must distinguish between α_1 in the text (defined between 0 and π) and $\tilde{\alpha}_1$ (defined between 0 and 2π); with this distinction in mind, it is easy to show that Eq. (F4) is the same as (2.4b) and Eq. (F5) is trivially the same as Eq. (2.4c).

APPENDIX G. STANDARD FORMS FOR 2×2 MATRICES

Given any 2×2 matrix $\mathbf{K}$ with $\det\mathbf{K}=1$, there exists a phase-space rotation of $\mathbf{K}$,

$$\mathbf{K}'=\mathbf{R}\mathbf{K}\mathbf{R}^{-1}, \qquad \mathbf{R}=\begin{bmatrix} \cos\chi & -\sin\chi \\ +\sin\chi & \cos\chi \end{bmatrix} \tag{G1}$$

such that $K'_{11}=K'_{22}$. The corresponding rotated coordinates

$$\begin{bmatrix} \sigma' \\ p'_\sigma \end{bmatrix}=\mathbf{R}\begin{bmatrix} \sigma \\ p_\sigma \end{bmatrix} \tag{G2}$$

are the principal axes of the invariant curves of the mapping by $\mathbf{K}$. The angle χ is given by

$$\tan(2\chi)=\frac{K_{11}-K_{22}}{K_{12}+K_{21}} \tag{G3}$$

Actually there are four rotation angles $\{\chi+n\pi/2 \mid n=-1,0,1,2\}$ which accomplish this. The principal axes can be further transformed by a canonical stretch,

$$\mathbf{K}''=\mathbf{S}\mathbf{K}'\mathbf{S}^{-1} \tag{G4}$$

where

$$\mathbf{S}=\begin{bmatrix} s & 0 \\ 0 & s^{-1} \end{bmatrix} \tag{G5}$$

and the parameter s is chosen to make $|K''_{12}|=|K''_{21}|$ (by convention $s>0$).

1. If $|\mathrm{Tr}\,\mathbf{K}| < 2$, then:

a. Since $\det \mathbf{K}'' = 1$, $\mathrm{sgn}\, K''_{12} = -\mathrm{sgn}\, K''_{21}$ and the matrix has the form $\left(\begin{smallmatrix} a & b \\ -b & a \end{smallmatrix}\right)$ with $a^2 + b^2 = 1$.

b. Hence we can define $\tilde{\alpha}_1$ such that the matrix $\mathbf{K}''$ represents a pure rotation,

$$\mathbf{K}'' = \begin{bmatrix} \cos \tilde{\alpha}_1 & \sin \tilde{\alpha}_1 \\ -\sin \tilde{\alpha}_1 & \cos \tilde{\alpha}_1 \end{bmatrix} \tag{G6}$$

By convention we take $0 \leqslant \tilde{\alpha}_1 < 2\pi$, so the action of $\mathbf{K}''$ on a point is to rotate that point in a clockwise sense.

c. Furthermore, the rotation $\mathbf{R}$ and stretch $\mathbf{S}$ preserve the signs of K_{12} and K_{21},

$$\begin{aligned} \mathrm{sgn}\, K_{12} = \mathrm{sgn}\, K'_{12} = \mathrm{sgn}\, K''_{12} &= -\mathrm{sgn}\, K_{21} \\ &= -\mathrm{sgn}\, K'_{21} = -\mathrm{sgn}\, K''_{21} \end{aligned} \tag{G7}$$

Proof: if $\mathbf{K}''$ in Eq. (G6) is transformed to $\mathbf{MKM}^{-1}$, where M is any matrix having $\det \mathbf{M} = 1$, then the signs of K_{12} and K_{21} are unchanged.

d. Therefore $\tilde{\alpha}_1$ is related to $\mathbf{K}$ by the formula

$$2 \cos \tilde{\alpha}_1 = \mathrm{Tr}\, \mathbf{K} \tag{G8a}$$

with

$$\begin{aligned} 0 < \tilde{\alpha}_1 < \pi \qquad & \text{if} \quad K_{12} > 0 \\ \pi < \tilde{\alpha}_1 < 2\pi \qquad & \text{if} \quad K_{12} < 0 \end{aligned} \tag{G8b}$$

2. If $|\mathrm{Tr}\,\mathbf{K}| > 2$, then:

a. There exists a choice of χ (i.e., a choice of $n = -1, 0, 1, 2$) such that the rotation preserves the sign of K_{12}. Presuming that K_{12} is not zero, then we can either choose χ between 0 and $\pi/2$ *or* between $-\pi/2$ and 0; for one of these choices the sign of K_{12} will not change as the rotation is performed. (See Fig. 12.)

b. Then since $\det \mathbf{K}'' = 1$, the matrix has the form $\left[\begin{smallmatrix} a & b \\ b & a \end{smallmatrix}\right]$, and $a^2 - b^2 = 1$. Therefore there exists a $\beta_1 > 0$ such that

$$\mathbf{K}'' = \begin{bmatrix} s_1 \cosh \beta_1 & s_2 \sinh \beta_1 \\ s_2 \sinh \beta_1 & s_1 \cosh \beta_1 \end{bmatrix} \tag{G9}$$

i.e., $\mathbf{K}''$ is a hyperbolic rotation. If $s_1 < 0$, then it is hyperbolic with reflection.

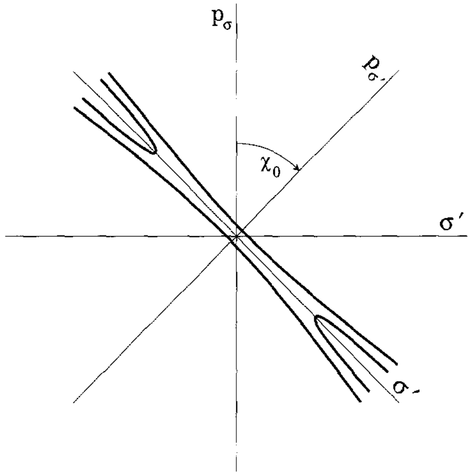

Fig. 12. Invariant curves for mapping around an unstable orbit, and rotation to a selected principal-axis frame. The principal axes are chosen such that (1) the p_σ and p'_σ axes pass through the same branch of the hyperbola and (2) the sign of K_{12} is not changed by the rotation. These two conditions are equivalent.

c. β_1, s_1, and s_2 can be determined from the rules

$$\begin{aligned} 2\cosh\beta_1 &= |\mathrm{Tr}\,\mathbf{K}|, \qquad \beta_1 > 0 \\ s_1 &= \mathrm{sgn}\,K_{11} \\ s_2 &= \mathrm{sgn}\,K_{12} \end{aligned} \tag{G10}$$

The product $s_1 s_2$ determines the sense of the hyperbolic rotation (Appendix F and Fig. 11).

Our choice of χ prevents the p_σ axis from passing through an asymptote (separatrix) while the rotation is carried out. The rotation angle is chosen from the four available such that the positive p'_σ axis passes through the same branch of the hyperbola as does the positive p_σ axis.

APPENDIX H. SYMMETRIES AND THEIR CONSEQUENCES

Let initial conditions be given as (p^i_u, p^i_v, u^i, v^i); assume Hamilton's canonical equations are integrated forward in time for a time T; let the final phase space point be (p^f_u, p^f_v, u^f, v^f). Let us abbreviate this sentence by the formula

$$(p^i_u, p^i_v, u^i, v^i) \xrightarrow{T} (p^f_u, p^f_v, u^f, v^f) \tag{H1}$$

If the Hamiltonian has inversion symmetry though the origin in momentum space, then by reversing the final momenta, treating them as initial conditions, and again integrating *forward* in time for the same duration T, the new final phase-space point will be the initial phase-space point with momenta reversed:

$$H(-p_u, -p_v, u, v) = H(p_u, p_v, u, v) \tag{H2}$$

implies

$$(-p_u^{\mathrm{f}}, -p_v^{\mathrm{f}}, u^{\mathrm{f}}, v^{\mathrm{f}}) \xrightarrow{T} (-p_u^{\mathrm{i}}, -p_v^{\mathrm{i}}, u^{\mathrm{i}}, v^{\mathrm{i}}) \tag{H3}$$

This symmetry is popularly known as "time-reversal invariance."

If the Hamiltonian has an analogous inversion symmetry in configuration space, we obtain

$$H(p_u, p_v, -u, -v) = H(p_u, p_v, u, v) \tag{H4}$$

implies

$$(p_u^{\mathrm{f}}, p_v^{\mathrm{f}}, -u^{\mathrm{f}}, -v^{\mathrm{f}}) \xrightarrow{T} (p_u^{\mathrm{i}}, p_v^{\mathrm{i}}, -u^{\mathrm{i}}, -v^{\mathrm{i}}) \tag{H5}$$

Under this condition, any orbit which is closed at the origin with return time T is periodic with period $2T$.

An analogous symmetry in the (p_u, u) Poincaré plane gives a different result

$$H(-p_u, p_v, -u, v) = H(p_u, p_v, u, v) \tag{H6}$$

implies

$$(-p_u^{\mathrm{i}}, p_v^{\mathrm{i}}, -u^{\mathrm{i}}, v^{\mathrm{i}}) \xrightarrow{T} (-p_u^{\mathrm{f}}, p_v^{\mathrm{f}}, -u^{\mathrm{f}}, v^{\mathrm{f}}) \tag{H7}$$

A corresponding result holds for inversion in the (p_v, v) Poincaré plane (Fig. 13).

In the applications of interest to us, the Hamiltonian has four independent reflection symmetries

$$H(\pm p_u, \pm p_v, \pm u, \pm v) = H(p_u, p_v, u, v) \tag{H8}$$

which imply all the symmetries above. In addition, the Hamiltonian is quadratic in the momenta. As a consequence, a Poincaré "half-map" can be defined. Starting from $u^i = 0$, we may integrate forward in time until the orbit again passes through $u = 0$ with either sign of p_u. As a special case of

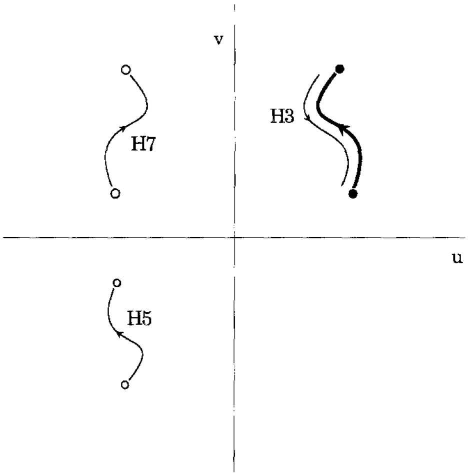

Fig. 13. Effect of symmetries of the Hamiltonian on orbits in configuration space. A given orbit is shown as the heavy line. Under the symmetry (H3) reversal of the final momentum makes the orbit retrace itself. Spatial inversion symmetry (H5) ensures the existence of another orbit in the third quadrant, while the symmetry (H7) ensures the existence of a reflected orbit in the second quadrant.

(H7), the mapping from $(p_v^{\mathrm{i}}, v^{\mathrm{i}})$ to $(p_v^{\mathrm{f}}, v^{\mathrm{f}})$ does not depend upon the sign of p_u:

$$(p_u^{\mathrm{i}}, p_v^{\mathrm{i}}, 0, v^{\mathrm{i}}) \to (p_u^{\mathrm{f}}, p_v^{\mathrm{f}}, 0, v^{\mathrm{f}}) \Rightarrow (-p_u^{\mathrm{i}}, p_v^{\mathrm{i}}, 0, v^{\mathrm{i}}) \to (-p_u^{\mathrm{f}}, p_v^{\mathrm{f}}, 0, v^{\mathrm{f}}) \qquad \text{(H9)}$$

As a consequence of this and the other symmetries (H8), the resulting map has a fourfold symmetry (Fig. 14),

$$(p_v^{\mathrm{i}}, v^{\mathrm{i}}) \to (p_v^{\mathrm{f}}, v^{\mathrm{f}}) \qquad \text{(H10a)}$$

implies

$$(-p_v^{\mathrm{f}}, v^{\mathrm{f}}) \to (-p_v^{\mathrm{i}}, v^{\mathrm{i}}) \qquad \text{(H10b)}$$

and

$$(p_v^{\mathrm{f}}, -v^{\mathrm{f}}) \to (p_v^{\mathrm{i}}, -v^{\mathrm{i}}) \qquad \text{(H10c)}$$

so

$$(-p_v^{\mathrm{i}}, -v^{\mathrm{i}}) \to (-p_v^{\mathrm{f}}, -v^{\mathrm{f}}) \qquad \text{(H10d)}$$

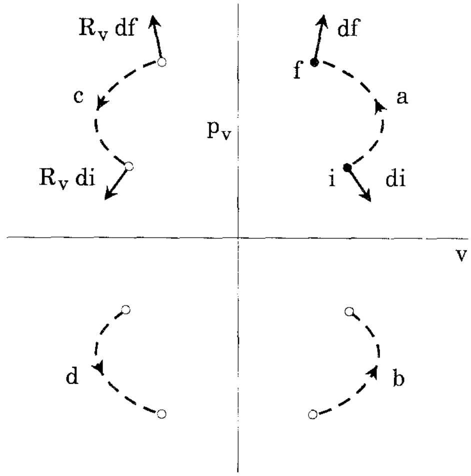

Fig. 14. Effect of the full set of symmetries of the Hamiltonian on the Poincaré half-map. Suppose a point **i** maps to **f**, indicated by the dashed curve *a*. Equations (H10b)–(H10d) are indicated by the dashed curves *b*, *c*, and *d*. The reflections of **f** map to reflections of **i**, and the inversion of **i** maps of the inversion of **f**. Likewise, for any small vector increment $d\mathbf{i}$, the point $\mathbf{i}+d\mathbf{i}$ maps to $\mathbf{f}+d\mathbf{f}$. A reflection of $d\mathbf{i}$ and $d\mathbf{f}$ is also drawn.

APPENDIX I. PROOF OF EQ. (2.6)

Let us rewrite Eq. (H10a) in the form

$$M(v, p_v) = (v', p_v') \tag{I1}$$

The derivative of this map at any point (v, p_v) is represented in the usual way by the Jacobian matrix

$$[\mathbf{J}(v, p_v)] \begin{bmatrix} dv \\ dp_v \end{bmatrix} = \begin{bmatrix} dv' \\ dp_v' \end{bmatrix} \tag{I2}$$

The symmetry represented by Eq. (H10c) is written as

$$M(-v', p_v') = (-v, p_v) \tag{I3}$$

and the corresponding derivative is

$$[\mathbf{J}(-v', p_v')] \begin{bmatrix} -dv' \\ dp_v' \end{bmatrix} = \begin{bmatrix} -dv \\ dp_v \end{bmatrix} \tag{I4}$$

We define $\mathbf{R}_v$ as the 2×2 reflection matrix $\left[\begin{smallmatrix}-1 & 0\\ 0 & 1\end{smallmatrix}\right]$. It acts only in this "tangent space"

$$\mathbf{R}_v\begin{bmatrix} dv \\ dp_v \end{bmatrix} = \begin{bmatrix} -dv \\ dp_v \end{bmatrix}$$

changing the sign of dv (but leaving the sign of v unchanged). Then

$$\mathbf{R}_v\mathbf{J}(-v', p'_v)\mathbf{R}_v\begin{bmatrix} dv' \\ dp'_v \end{bmatrix} = \begin{bmatrix} dv \\ dp_v \end{bmatrix} \tag{I5}$$

so

$$\mathbf{J}(-v', p'_v) = \mathbf{R}_v[\mathbf{J}(v, p_v)]^{-1}\mathbf{R}_v \tag{I6a}$$

By a similar method, we can prove that

$$\mathbf{J}(v', -p'_v) = \mathbf{R}_p[\mathbf{J}(v, p_v)]^{-1}\mathbf{R}_p \tag{I6b}$$

Consider any orbit which is closed at the origin, so $v = v' = 0$; it starts at p_v and ends at p'_v. The Jacobian matrix for the second cycle of this orbit is

$$\mathbf{J}(0, p'_v) = \mathbf{R}_v[\mathbf{J}(0, p_v)]^{-1}\mathbf{R}_v \tag{I7}$$

Writing the Jacobian matrix for the first cycle in the usual way

$$\mathbf{J}(0, p_v) = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} \tag{I8}$$

we obtain the matrix for the second cycle as

$$\mathbf{J}(0, p'_v) = \begin{bmatrix} J_{22} & J_{12} \\ J_{21} & J_{11} \end{bmatrix} \tag{I9}$$

This is Eq. (2.6).

For an orbit of type 1, if $p'_v = p_v$, the Jacobian matrix on the second cycle must be identical to that of the first cycle. Hence

$$J_{11} = J_{22} \tag{I10}$$

Using the symmetry (I6b), we can prove that this equation also holds for orbits with $p'_v = -p_v$. (It does not hold for type 2.)

Similar relationships hold for the matrix **K**. They follow from the fact that the effective force-constant $k_\sigma(t)$ in Eq. (E.2) has the symmetry

$$k_\sigma(T+t) = k_\sigma(T-t) \tag{I11}$$

Using this property and the differential equations (E2), one can show that (1) the matrix **K** for the second closure is the matrix for the first closure with the diagonal elements exchanged, (2) if we start a phase point on the positive p_σ axis at $t = 0$ and follow its motion through one closure to T, and then if we start another phase point on the positive p_σ axis at T and follow its motion to $2T$, the two points will not necessarily end at the same spot, but they will have completed the same number of full revolutions and the same number of half-revolutions. Hence the Maslov index for the first closure of the second half of the orbit is the same as the Maslov index for the first closure of the first half of the orbit. Also, the change in the Maslov index on any closure is always either μ_1 or $\mu_1 + 1$.

APPENDIX J. PROOF OF EQ. (2.8)

For systems with reflection symmetries, the second closure of an orbit closed at the origin, of either type 1 or type 2, is a period of the orbit. The Jacobian matrix for the second closure is, according to Eqs. (2.6a) and (2.6b),

$$\mathbf{J}(2) \equiv \mathbf{J}'\mathbf{J} = \begin{pmatrix} 2J_{11}J_{22} - 1 & 2J_{12}J_{22} \\ 2J_{21}J_{11} & 2J_{11}J_{22} - 1 \end{pmatrix} \tag{J1}$$

Here the diagonal elements of $\mathbf{J}(2)$ are equal to each other. For even closures of the orbit, the Jacobian matrix $\mathbf{J}(n\,\text{even})$ is simply the $(n/2)$th self-multiplication of $\mathbf{J}(2)$. According to Eq. (C12), we have

$$\mathbf{J}(n\,\text{even}) = \begin{bmatrix} C_{n/2} & 2J_{12}J_{22}D_{n/2-1} \\ 2J_{21}J_{11}D_{n/2-1} & C_{n/2} \end{bmatrix} \tag{J2}$$

where C_m and D_m are the Chebyshev polynomials of the first kind and the second kind, with $\cos 2\alpha_1'$ as the variable of the polynomials, where α_1' is defined such that

$$\cos\alpha_1' = s'(J_{11}J_{22})^{1/2}, \qquad s' \equiv \mathrm{sgn}(J_{11} + J_{22}), \qquad \text{if} \quad 0 < J_{11}J_{22} < 1$$

$$\cos(2\alpha_1') = s(2J_{11}J_{22} - 1), \qquad s \equiv \mathrm{sgn}(J_{11}J_{22}), \qquad \text{otherwise} \tag{J3}$$

Here α_1' is real $(0 < \alpha_1' < \pi)$ if $0 < J_{11}J_{22} < 1$, and α_1' is positive imaginary otherwise. In terms of α_1', the diagonal elements of $\mathbf{J}(2)$ in Eq. (J1) become, in either case,

$$2J_{11}J_{22} - 1 = s\cos(2\alpha_1') \tag{J4}$$

For odd repetitions of the closed orbit, Eq. (J2) can be used to determine the expression for the Jacobian matrix $\mathbf{J}(n \text{ odd})$, and the result is

$$\mathbf{J}(n \text{ odd}) = \mathbf{J}\mathbf{J}(n-1, \text{even})$$
$$= \begin{bmatrix} J_{11}(D_{(n-1)/2} - D_{(n-3)/2}) & J_{12}(D_{(n-1)/2} + D_{(n-3)/2}) \\ J_{21}(D_{(n-1)/2} + D_{(n-3)/2} & J_{22}(D_{(n-1)/2} - D_{(n-3)/2}) \end{bmatrix} \quad \text{(J5)}$$

We then use the properties of the Chebyshev polynomials, Eqs. (C6) and (C17), to arrive at the following results:

$$\mathbf{J}(n \text{ even}) = s^{n/2-1} \begin{pmatrix} s\cos(n\alpha_1') & 2J_{12}J_{22}\dfrac{\sin(n\alpha_1')}{\sin(2\alpha_1')} \\ 2J_{21}J_{11}\dfrac{\sin(n\alpha_1')}{\sin(2\alpha_1')} & s\cos(n\alpha_1') \end{pmatrix} \quad \text{(J6a)}$$

and

$$\mathbf{J}(n \text{ odd}) = \mathbf{J}\mathbf{J}(n-1) = s^{(n-1)/2} \begin{pmatrix} J_{11}\dfrac{\cos(n\alpha_1')}{\cos\alpha_1'} & J_{12}\dfrac{\sin(n\alpha_1')}{\sin\alpha_1'} \\ J_{21}\dfrac{\sin(n\alpha_1')}{\sin\alpha_1'} & J_{22}\dfrac{\cos(n\alpha_1')}{\cos\alpha_1'} \end{pmatrix} \quad \text{(J6b)}$$

Equation (2.8) follows immediately.

The Maslov index for the nth repetition of a closed orbit is the number of singularities of the semiclassical amplitude, which is inversely proportional to the square root of $J_{12}(z)$, when the continuous variable z goes from 0^+ to n. Hence the Maslov index can be counted by monitoring the number of sign changes of $J_{12}(n)$, that is, the number of zeros of $J_{12}(n)$. Equations (J6a) and (J6b) give explicit expressions for $J_{12}(n)$, and therefore can be used to count the Maslov index. The result of this counting is listed in Eq. (2.10). An equivalent approach giving the same result together with additional details is given in Appendix K.

The results shown in this Appendix are all true for either type 1 or type 2 orbits. For type 1 orbits (i.e., $J_{11} = J_{22}$), α_1' is equal to the winding angle α_1 if the orbit is stable and $\alpha_1' = i\beta_1$ if unstable, where β_1 is the (positive) Lyapunov exponent. For stable type 1 orbits, $s = +1$, and Eqs. (J6a) and (J6b) can be combined to one formula,

$$\mathbf{J}(n) = \mathbf{J}^n = \begin{bmatrix} \cos(n\alpha_1) & J_{12}\dfrac{\sin(n\alpha_1)}{\sin\alpha_1} \\ J_{21}\dfrac{\sin(n\alpha_1)}{\sin\alpha_1} & \cos(n\alpha_1) \end{bmatrix}, \quad \text{stable} \quad \text{(J7)}$$

which is the same as Eq. (C18a). For an unstable type 1 orbit (i.e., $J_{11}=J_{22}$ and $|J_{11}|>1$), $J_{11}=J_{22}=s'\cosh\beta_1$, and Eqs. (J6a) and (J6b) become Eq. (C18b), as expected.

APPENDIX K. Maslov Index for Repetitions of Closed Orbits

A more explicit method to find the Maslov index for subsequent returns of a closed orbit follows the same reasoning as in Appendix F. We could monitor $\sigma(t)$, $J_{sc}(t)$, or $K_{12}(t)$ as functions of time along the trajectory; μ_n will then be the number of times these quantities change sign between $t=0$ and $t=nT$, where T is now the closure time of the orbit.

If the orbit is of type 1, then the period of the force constant $k_\sigma(t)$ in Eq. (E2) is equal to the closure time for the orbit. Each closure then constitutes a period of $k_\sigma(t)$, so we can treat such orbits as if they were periodic with period T. Therefore Eqs. (F4) or (F5) hold with n being the label for the closure. There is only one important difference: the relationship between **K** and **J** for closed orbits is

$$\mathbf{K}=\begin{bmatrix}-\cos\Theta_f & 0\\ 0 & 1/(-\cos\Theta_f)\end{bmatrix}\mathbf{J}\begin{bmatrix}1/\cos\Theta_i & 0\\ 0 & \cos\Theta_i\end{bmatrix} \tag{K1}$$

Recall that Θ_i is the direction that the orbit goes out from the origin and Θ_f is the direction from which the orbit returns.

If the orbit is type 2, then the period of the force constant $k_\sigma(t)$ is twice the closure time. However, the force constant has the symmetry (I.11). Therefore we can still obtain a simple formula for the Maslov index on any return using formulas analogous to those in Appendix J.

Assume the orbit is stable; the condition for this is $0<K_{11}K_{22}<1$. Define the angle $\tilde{\alpha}_1'$ such that

$$\cos\tilde{\alpha}_1'=\tilde{s}(K_{11}K_{22})^{1/2}=\tilde{s}(J_{11}J_{22})^{1/2},\qquad \tilde{s}=\operatorname{sgn}(K_{11}+K_{22}) \tag{K2}$$

with the convention

$$0<\tilde{\alpha}_1'<\pi \qquad \text{if} \quad K_{12}>0$$

$$\pi<\tilde{\alpha}_1'<2\pi \qquad \text{if} \quad K_{12}<0$$

Then, defining $a=(K_{11}/K_{22})^{1/2}$ and $b=(-K_{12}/K_{21})^{1/2}$ with positive square roots, the matrix K has the form

$$\mathbf{K}=\begin{bmatrix}a\cos\tilde{\alpha}_1' & b\sin\tilde{\alpha}_1'\\ -(1/b)\sin\tilde{\alpha}_1' & (1/a)\cos\tilde{\alpha}_1'\end{bmatrix} \tag{K3}$$

Then for any even closure

$$\mathbf{K}(n) = [\mathbf{K}'(1)\,\mathbf{K}(1)]^{n/2} = \begin{bmatrix} \cos(n\tilde{\alpha}'_1) & (b/a)\sin(n\tilde{\alpha}'_1) \\ -(a/b)\sin(n\tilde{\alpha}'_1) & \cos(n\tilde{\alpha}'_1) \end{bmatrix} \qquad \text{(K4)}$$

and for any odd closure

$$\mathbf{K}(n) = \mathbf{K}(1)[\mathbf{K}'(1)\,\mathbf{K}(1)]^{(n-1)/2}$$

$$= \begin{bmatrix} a\cos(n\tilde{\alpha}'_1) & b\sin(n\tilde{\alpha}'_1) \\ -(1/b)\sin(n\tilde{\alpha}'_1) & (1/a)\cos(n\tilde{\alpha}'_1) \end{bmatrix} \qquad \text{(K5)}$$

The change in the Maslov index on each return is twice the number of full revolutions of the phase point on the first return (again full revolutions are hidden by the strobing) plus the number of sign changes of K_{12} that are explicitly contained in Eqs. (K4) and (K5)—i.e., the number of changes of sign of the function $\sin(z\alpha'_1)$ between $z = n-1$ and $z = n$. Hence

$$\mu_n = 2n\,\mathrm{Int}\,\frac{\mu_1}{2} + \mathrm{Int}\,\frac{n\tilde{\alpha}'_1}{\pi} \qquad \text{(K6)}$$

Again bearing in mind the distinction between $\tilde{\alpha}'_1$ and α'_1 (the former describing $\mathbf{K}$ and the latter describing $\mathbf{J}$), it is easy to show that (K6) is equivalent to the first two lines of (2.10).

If the orbit is unstable, several cases arise. Suppose $K_{11}K_{22} > 1$. Define β'_1 and a new a and b such that

$$\begin{aligned} \cosh\beta'_1 &= |K_{11}K_{22}|^{1/2}, \qquad \beta'_1 > 0 \\ a &= |K_{11}/K_{22}|^{1/2} \\ b &= |K_{12}/K_{21}|^{1/2} \\ s_1 &= \mathrm{sgn}\,K_{11} \\ s_2 &= \mathrm{sgn}\,K_{12} \end{aligned} \qquad \text{(K7)}$$

where β'_1, a, and b are all taken to be positive. Then it is easy to verify that

$$\mathbf{K}(1) = \begin{bmatrix} s_1 a\cosh(n\beta'_1) & s_2 b\sinh(n\beta'_1) \\ (s_2/b)\sinh(n\beta'_1) & (s_1/a)\cosh(n\beta'_1) \end{bmatrix}$$

$$\mathbf{K}(n) = [\mathbf{K}'\mathbf{K}]^{n/2} = \begin{bmatrix} \cosh(n\beta'_1) & s_1 s_2 (b/a)\sinh(n\beta'_1) \\ s_1 s_2 (a/b)\sinh(n\beta'_1) & \cosh(n\beta'_1) \end{bmatrix} \qquad \text{(K8)}$$

$$\mathbf{K}(n+1) = \mathbf{K}[\mathbf{K}'\mathbf{K}]^{n/2} = \begin{bmatrix} s_1 a\cosh[(n+1)\beta'_1] & s_2 b\sinh[(n+1)\beta'_1] \\ (s_2/b)\sinh[(n+1)\beta'_1] & (s_1/a)\cosh[(n+1)\beta'_1] \end{bmatrix}$$

These formulas presume that n is even.

In this case the even repetitions of the orbit are pure hyperbolic rotations and the sense of the rotations is given by the product $s_1 s_2$. If $s_1 > 0$, the odd returns also correspond to pure hyperbolic rotation, while if $s_1 < 0$ the even and odd returns alternate in the manner of a hyperbolic rotation with reflection. By counting the changes of sign of $K_{12}(n)$ we find

$$\begin{aligned} \mu_n &= n\mu_1 && \text{if} \quad K_{11}K_{22} > 1, \quad s_1 s_2 > 0 \\ \mu_n &= n\mu_1 + n - 1 && \text{if} \quad K_{11}K_{22} > 1, \quad s_1 s_2 < 0 \end{aligned} \tag{K9}$$

Finally, if $K_{11}K_{22} < 0$, we use the same definitions (K7), and we find

$$\mathbf{K}(1) = \begin{bmatrix} s_1 a \cosh(n\beta'_1) & s_2 b \sinh(n\beta'_1) \\ -(s_2/b)\sinh(n\beta'_1) & -(s_1/a)\cosh(n\beta'_1) \end{bmatrix}$$

$$\mathbf{K}(n) = [\mathbf{K}'\mathbf{K}]^{n/2} = (-)^{n/2} \begin{bmatrix} \cosh(n\beta'_1) & s_1 s_2 (b/a)\sinh(n\beta'_1) \\ s_1 s_2 (a/b)\sinh(n\beta'_1) & \cosh(n\beta'_1) \end{bmatrix}$$

$$\begin{aligned} \mathbf{K}(n+1) &= \mathbf{K}[\mathbf{K}'\mathbf{K}]^{n/2} \\ &= (-)^{n/2} \begin{bmatrix} s_1 a \cosh[(n+1)\beta'_1] & s_2 b \sinh[(n+1)\beta'_1] \\ -(s_2/b)\sinh[(n+1)\beta'_1] & -(s_1/a)\cosh[(n+1)\beta'_1] \end{bmatrix} \end{aligned} \tag{K10}$$

again presuming n is even.

Even repetitions are hyperbolic rotations with reflection. Again the sense of rotation is given by $s_1 s_2$. Odd repetitions occupy the quadrants in the (σp_σ) plane that are not occupied by even repetitions. Recalling that the continunous motion of the phase point can only cross the p_σ axis in a clockwise sense, one finds that

$$\begin{aligned} \mu_n &= n\mu_1 + \operatorname{Int}\frac{n}{2} && \text{if} \quad K_{11}K_{22} < 0, \quad s_1 s_2 > 0 \\ \mu_n &= n\mu_1 + \operatorname{Int}\frac{n-1}{2} && \text{if} \quad K_{11}K_{22} < 0, \quad s_1 s_2 < 0 \end{aligned} \tag{K11}$$

APPENDIX L. ORBITS WITH ENDPOINTS

In all of the above, we have assumed that the periodic orbit has no endpoints. However, orbits of type 1b do have endpoints, so some additional discussion is needed for them.

The assumed form of the Hamiltonian implies time-reversal symmetry, so any orbit with an endpoint exactly retraces itself, and if it is periodic it must have a second endpoint, as in Fig. 1b. We may define $\Lambda = 0$ to be either endpoint (the "initial" one) and let $\Lambda(t)$ increase up to the second endpoint (the "final" one). The coordinates λ and σ can then be defined using Eqs. (D1)–(D5) from one endpoint to the other. The unit vector $\hat{\lambda}$ points along the orbit from the "initial" endpoint to the "final" endpoint. It is *not* useful to define the coordinates (λ, σ) so that they turn around at the final endpoint. Instead, $d\lambda/dt$, and $K(p_\sigma, \sigma; \lambda)$ go from positive through zero to negative at the final endpoint.

Then all of the equations in Appendix D are valid except at the endpoints. There $d\sigma/d\lambda$ and $dp_\sigma/d\lambda$ have singularities associated with the quantity $P_\Lambda(\lambda)$ in the denominator of Eq. (D12a). These are integrable singularities, however, and, through appropriate mumbling about the treatment of these singularities, one can again arrive at Hill's equations (D12b) and (E2).

The semiclassical Jacobian (E3) passes through zero whenever $\dot{\Lambda}(t) = 0$, which happens at each endpoint, or whenever $\sigma(t) = 0$. It is most convenient to count these points separately: the matrix $\mathbf{K}(t)$ in Eq. (E5) can still be used to count zeros of $\sigma(t)$, and we then add 1 to the Maslov index every time the trajectory touches an endpoint.

Equation (F6) describes the relationship between $\mathbf{K}$ and $\mathbf{J}$, and the rest of the formulas in Appendices F and G describe the behavior of iterates of $\mathbf{K}$.

Net result: Treat case 1b like case 1a, but add 1 to μ_1 as the contribution from the endpoint. Then Eq. (2.4a), containing $n\mu_1$, includes the contributions of successive endpoints.

APPENDIX M. DOUBLE-COUNTING FOR ZERO-DEGREE ORBITS

We give two arguments for double-counting passages through the zero-degree orbit.

1. In general the full semiclassical Jacobian is given by

$$J_{sc} = \frac{\partial(x, y, z)}{\partial(t, \theta^0, \phi^0)} = \rho(t) \frac{\partial(\rho, z, \phi)}{\partial(t, \theta^\circ, \phi^0)}$$

By further changes of variable, from (ρ, z) to (u, v) to (λ, σ), we find that the semiclassical Jacobian contains the factors $\rho(t)\,\dot{\Lambda}(t)\,\sigma(t)$ (cf. Appendix E). Each factor can pass through zero, and each then causes the Maslov index to increase by 1. When a neighbor passes through an orbit on the z axis, both $\rho(t)$ and $\sigma(t)$ vanish simultaneously, but each still contributes 1 for a total of 2.

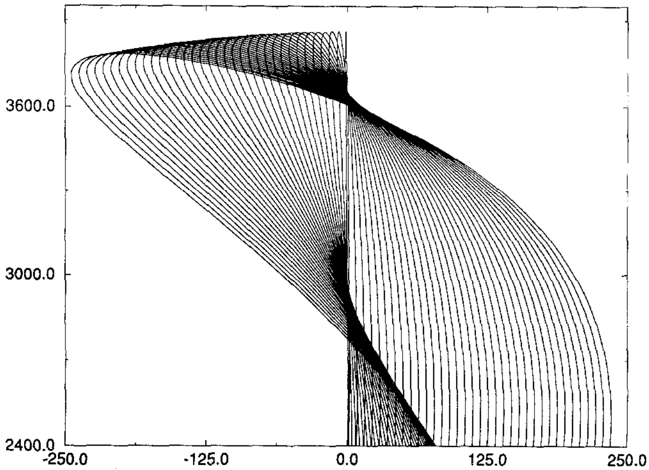

Fig. 15. Zero-degree orbit and its friends for the diamagnetic Kepler problem. The outermost of these is traveling up on the right; it encounters a caustic $(+1)$, then crosses over the z axis toward the left $(+1)$, encounters the caustic associated with the endpoint of the parallel orbit $(+1)$, then crosses the z axis again $(+1)$, and then another caustic on its way down $(+1)$. For the innermost neighbor, each z-axis crossing coincides with a caustic, and therefore counts $+2$. The endpoint is still $+1$.

2. Figure 15 shows the upper end of the zero-degree orbit and its neighbors, calculated by solving exact equations of motion (not linearized equations). For the most distant neighbors, it is evident that passage through a caustic and passage through the z axis are distinct events, each contributing 1 to the Maslov index. For the close neighbors, and particularly in the linear approximation, the caustic and the z axis coincide. However, the zero-degree orbit and all its neighbors constitute a single Lagrangian manifold, and each regular domain of the manifold has a unique Maslov index. Equivalently, the phase of the semiclassical wavefunction associated with each regular domain is well-defined, and the phase at the zero-degree orbit is the limit of the phase of the neighbors. Therefore we add 2 for each crossing of the zero-degree orbit by its neighbors.

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