# Uniform semiclassical approximations for umbilic bifurcation catastrophes

Jörg Main and Günter Wunner
*Institut für Theoretische Physik I, Ruhr-Universität Bochum, D-44780 Bochum, Germany*
(Received 5 August 1997; revised manuscript received 5 February 1998)

Gutzwiller's trace formula for the semiclassical density of states diverges at the bifurcation points of periodic orbits, and has to be replaced with uniform semiclassical approximations. We present a method to derive these expressions from the standard representations of the elementary catastrophes, and to relate the uniform solutions directly to classical periodic orbit parameters, thereby circumventing the numerical application of normal form theory. The technique allows an easy handling of ungeneric bifurcations with corank 2 such as the umbilic catastrophes, and is demonstrated on a hyperbolic umbilic in the diamagnetic Kepler problem. [S1063-651X(98)15306-0]

PACS number(s): 05.45.+b, 03.65.Sq, 32.60.+i

Gutzwiller's periodic orbit theory [1,2] has become the key for a semiclassical interpretation of quantum systems with underlying chaotic classical dynamics. The contributions of isolated periodic orbits to the periodic orbit sum are given as

$$\mathcal{A}_{\rm po}=\frac{T_{\rm po}e^{i[S_{\rm po}/\hbar-(\pi/2)\mu_{\rm po}]}}{\sqrt{|\det(M_{\rm po}-I)|}}, \tag{1}$$

with $T_{\rm po}$, $S_{\rm po}$, $M_{\rm po}$, and $\mu_{\rm po}$ the orbital period, classical action, stability matrix, and Maslov index, respectively. However, Eq. (1) diverges at the bifurcation points of periodic orbits where orbits are not isolated, and Eq. (1) must be replaced with uniform approximations given in terms of diffraction catastrophe integrals [3,4]. The study of bifurcations and uniform approximations is of fundamental importance to a complete understanding and semiclassical treatment of systems with mixed regular-chaotic classical dynamics [5]. The derivation of uniform solutions based on a canonical transformation of the coordinates and momenta to normal form coordinates [6,7] and the construction of diffraction integrals in terms of the new variables, is usually a lengthy and nontrivial task [3–5,8], especially in the neighborhood of bifurcations of codimension $K\geqslant 2$, and for catastrophes of corank 2 such as the umbilics. A simple scheme would be desirable to construct uniform approximations from classical periodic orbits, and to relate the parameters of catastrophe diffraction integrals directly to the periodic orbit parameters, such as the classical action $S$ and the eigenvalues of the stability matrix $M$.

In this paper we want to demonstrate that in practical applications the derivation of uniform semiclassical approximations can be considerably simplified, especially for ungeneric bifurcations of codimension $K\geqslant 2$ and catastrophes of corank 2 when starting directly from the standard representation of the elementary catastrophes [9,10]. We illustrate our method by way of example of the diamagnetic Kepler problem [11,12] given by the Hamiltonian [in atomic units, $\gamma=B/(2.35\times 10^5\mathrm{T})$, and $L_z=m\hbar=0$]

$$H=\frac{1}{2}\mathbf{p}^2-\frac{1}{r}+\frac{1}{8}\gamma^2\rho^2 \quad , \tag{2}$$

which is a scaling system, with $w=1/\hbar_{\rm eff}\equiv\gamma^{-1/3}$ the scaling parameter and $\tilde{E}\equiv E\gamma^{-2/3}$ the scaled energy. The classical dynamics is determined by the scaled energy $\tilde{E}$, but does not depend on $w$. We investigate the birth of four periodic orbits through two nearby bifurcations near the scaled energy $\tilde{E}\approx -0.096$, where we search for both real and complex ''ghost'' orbits [8,13]. For the nomenclature of the real orbits, we adopt the symbolic code of Ref. [14]. At scaled energy $\tilde{E}_b^{(1)}=-0.096\,89$, the two orbits $00+-$ and $++++---$ are born in a tangent bifurcation. At energies $\tilde{E}<\tilde{E}_b^{(1)}$, a prebifurcation ghost orbit and its complex conjugate exist in the complex continuation of the phase space. Orbit $00+-$ is born unstable, and turns stable at the slightly higher energy $\tilde{E}_b^{(2)}=-0.094\,51$. This is the bifurcation point of two additional orbits, $0-+--$ and its time reversal $0---+$, which also have ghost orbits as predecessors. The graphs of the real orbits at energy $E=0$ are shown as insets in Fig. 1, and the classical periodic orbit parameters are presented as solid lines in Figs. 1 and 2. Figure 1 shows the difference in scaled action, $\Delta\tilde{S}\equiv\Delta S/(2\pi w)$, between the orbits. The action of orbit $0-+--$ (or its time reversal $0---+$), which is also real for its prebifurcation ghost orbits, has been taken as the reference action.

At this point the usual procedure would be to investigate the classical dynamics in the neighborhood of the periodic orbits by numerical application of normal form theory [6,7]. The representation of the dynamics in normal form coordinates would finally lead to the correct type of catastrophe diffraction integral related to the uniform semiclassical approximation with numerically well determined coefficients. However, the numerical procedure of local canonical transformations to normal form coordinates, e.g., by means of local Fourier-Taylor series expansions with numerically obtained coefficients [7], is rather lengthy and tedious, especially for bifurcations related to catastrophes of higher codimension or corank. The main result of this paper is to demonstrate that there is a shortcut to the usual procedure which allows one to circumvent the numerical application of normal form theory. By our new method, an easy construction of uniform semiclassical approximations for ungeneric types of catastrophes, e.g., the umbilics, becomes feasible.

 

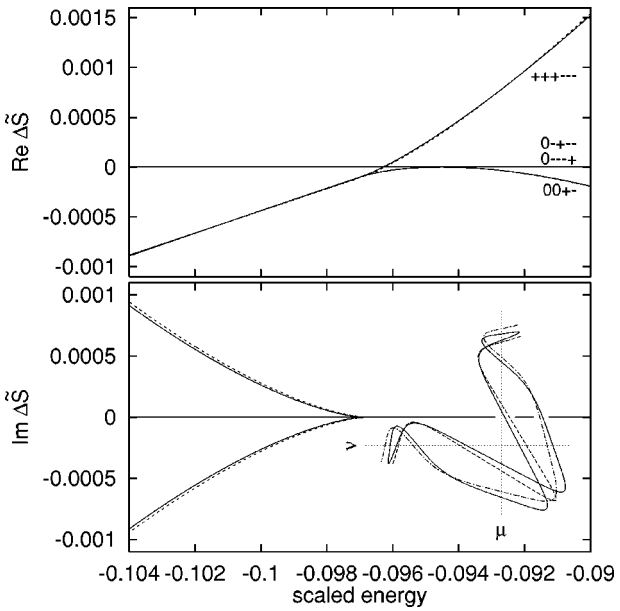


FIG. 1. Difference $\Delta\tilde{S}$ between the classical action of the four periodic orbits involved in the bifurcations. Dashed lines: Analytical fits related to the hyperbolic umbilic catastrophe. Inset: Graphs of periodic orbits $0-+--$ and its time reversals $0---+$ (solid line), $00+-$ (dashed line), and $+++---$ (dash-dotted line) drawn in semiparabolical coordinates $\mu=(r+z)^{1/2}$ and $\nu=(r-z)^{1/2}$.

Choosing the elementary catastrophe diffraction integrals as the ansatz for the uniform semiclassical approximation, we must be able to identify the stationary points of the exponents with the periodic orbits; i.e., in our example, four stationary points must exist. From the seven ''elementary catastrophes'' of Refs. [9,10], this is the case only for the swallowtail and the elliptic and hyperbolic umbilic. The correct choice in our example turns out to be the hyperbolic umbilic catastrophe, which is of importance, e.g., for uniform $S$ matrix approximations in semiclassical scattering theory [15]. It is a corank 2 catastrophe, i.e., the diffraction integral is two dimensional,

$$\Psi(x,y)=\int_{-\infty}^{+\infty}dp\int_{-\infty}^{+\infty}dq\ e^{i\Phi(p,q;x,y)} \tag{3}$$

with

$$\Phi(p,q;x,y)=p^3+q^3+y(p+q)^2+x(p+q)\quad . \tag{4}$$

For our convenience, the function $\Phi(p,q;x,y)$ slightly differs from the standard polynomial of the hyperbolic umbilic given in Ref. [10], but the diffraction integral (3) can be easily transformed to the standard representation. The four stationary points of integral (3) are readily obtained from the condition $\nabla\Phi=0$ as

$$p_0=-q_0=\pm\sqrt{-x/3}\Rightarrow\Phi(p_0,q_0;x,y)=0 \tag{5}$$

and

$$\begin{aligned}p_0=q_0&=-\frac{2}{3}y\pm\sqrt{\frac{4}{9}y^2-\frac{x}{3}}\\ \Rightarrow&\Phi(p_0,q_0;x,y)\\ &=\frac{4}{3}y\left(\frac{8}{9}y^2-x\right)\mp4\left(\frac{4}{9}y^2-\frac{x}{3}\right)^{3/2}\quad .\end{aligned} \tag{6}$$

The function $\Phi(p_0,q_0;x,y)$ must now be adapted to the classical action of the four periodic orbits, i.e., $\Delta S=2\pi w\Delta\tilde{S}\approx\Phi(p_0,q_0;x,y)$, which is well fulfilled for

$$x=aw^{2/3}(\tilde{E}-\tilde{E}_b^{(2)}),\quad y=bw^{1/3}\quad , \tag{7}$$

and constants $a=-5.415$ and $b=0.096\,65$, as can be seen from the dashed lines in Fig. 1. Note that the agreement holds for both the real and complex ghost orbits.

The next step to obtain the uniform solution is to calculate the diffraction integral (3) within the stationary phase approximation. For $\tilde{E}>\tilde{E}_b^{(2)}$, there are four real stationary points $(p_0,q_0)$ [see Eqs. (5) and (6)], and after expanding $\Phi(p,q;x,y)$ around the stationary points up to second order in $p$ and $q$, the diffraction integral becomes the sum of Fresnel integrals, viz.

$$\Psi(x,y)\overset{x\ll0}{\sim}\frac{2\pi}{\sqrt{-3x}}+\sum_{+,-}\frac{\pi e^{i\{(4/3)y[(8/9)y^2-x]\mp4[(4/9)y^2-x/3]^{3/2}\pm\pi/2\}}}{\sqrt{(4y^2-3x)\mp2y\sqrt{4y^2-3x}}}\ . \tag{8}$$

The terms of Eq. (8) can now be compared to the standard periodic orbit contributions (1) of Gutzwiller's trace formula. In our example, the first term is related to the orbit $0-+--$ (with a multiplicity factor of 2 for its time reversal $0---+$), and the other two terms are related to the orbits $00+-$ and $+++---$ for the upper and lower signs, re-

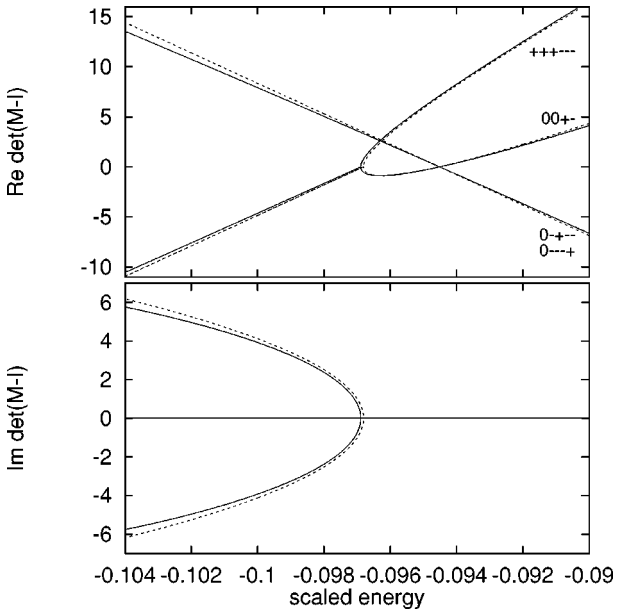


FIG. 2. Same as Fig. 1, but for the determinant $\det(M-I)$ of the periodic orbits.

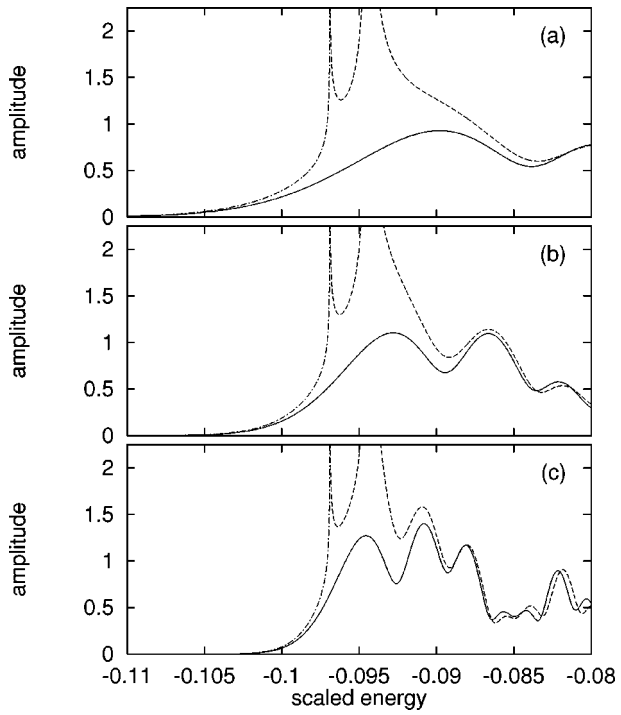


FIG. 3. Semiclassical amplitudes (absolute values) for magnetic-field strengths (a) $\gamma=10^{-7}$, (b) $\gamma=10^{-8}$, and (c) $\gamma=10^{-9}$ in units of the time period $T_0$. Dashed line: Amplitudes of the standard semiclassical trace formula. Dash-dotted line: Ghost orbit contribution. Solid line: Uniform approximation for the hyperbolic umbilic catastrophe.

spectively. The phase shift in the numerators describe the differences of the action $\Delta S$ and of the Maslov index $\Delta\mu=\mp 1$ relative to the reference orbit $0-+--$. The denominators are, up to a factor $cw^{1/3}$, with $c=0.1034$, the square root of $|\det(M-I)|$, with $M$ the stability matrix. Figure 2 presents the comparison for the determinants obtained from classical periodic orbit calculations (solid lines) and from Eqs. (7) and (8) (dashed lines). The agreement is very good for both the real and complex ghost orbits, similar to the agreement found for $\Delta\tilde{S}$ in Fig. 1. The constant $c$ introduced above determines the normalization of the uniform semiclassical approximation for the hyperbolic umbilic bifurcation, which is finally obtained as

$$\mathcal{A}_{\text{uniform}}(\tilde{E},w)=(c/\pi)T_0 w^{1/3} \times\Psi[aw^{2/3}(\tilde{E}-\tilde{E}_b^{(2)}),bw^{1/3}] \times e^{i[2\pi\tilde{S}_0 w-(\pi/2)\mu_0]}, \tag{9}$$

with $T_0$, $S_0$, and $\mu_0$ denoting the orbital period, action, and Maslov index of the reference orbit $0-+--$, and constants $a$, $b$, and $c$ as given above. Note that all parameters are readily determined by classical periodic orbit calculations.

The comparison between the conventional semiclassical trace formula (1) for isolated returning orbits and the uniform approximation (9) for the hyperbolic umbilic catastrophe is presented in Fig. 3 at the magnetic field strengths $\gamma=10^{-7}$, $10^{-8}$, and $10^{-9}$. For graphical purposes we suppress the highly oscillatory part resulting from the function $\exp(i[S_0/\hbar-(\pi/2)\mu_0])$ by plotting the absolute value of $\mathcal{A}(\tilde{E},w)$ instead of the real part. The dashed line in Fig. 3 is the superposition of the isolated periodic orbit contributions from the four orbits involved in the bifurcations. The modulations of the amplitude are caused by the constructive and destructive interference of the real orbits at energies $\tilde{E}>\tilde{E}_b^{(2)}$, and are most pronounced at low magnetic field strength [see Fig. 3(c)]. The amplitude diverges at the two bifurcation points. For the calculation of the uniform approximation (9), we numerically evaluated the catastrophe diffraction integral (3) using a more simple and direct technique as described in Ref. [16]. Details of our method, which is based on Taylor series expansions will be given elsewhere [17]. The solid line in Fig. 3 is the uniform approximation (9). It does not diverge at the bifurcation points, but decreases exponentially at energies $\tilde{E}<\tilde{E}_b^{(1)}$. At these energies no real orbits exist, and the amplitude in the standard formulation would be zero when only real orbits are considered. However, the exponential tail of the uniform approximation (9) is well reproduced by a ghost orbit [8,13] with a positive imaginary part of the complex action. As can be shown, the asymptotic expansion of the diffraction integral (3) has, for $x\gg 0$, exactly the form of Eq. (1), but with complex action $S$ and determinant $\det(M-I)$ [17]. The ghost orbit contribution is shown as dash-dotted line in Fig. 3.

To verify the hyperbolic umbilic catastrophe in quantum spectra, we diagonalized the Hamiltonian (2) in a complete basis set (for computational details see, e.g., Ref. [18]) at constant scaled energy $\tilde{E}=-0.1$, which is slightly below the bifurcation energies, and calculated 9715 eigenvalues $w_n$ for the scaling parameter in the region $w<140$. The scaled spectrum was analyzed by the high-resolution method of Ref. [19], i.e., the density of states $\varrho(w)=\Sigma_n\delta(w-w_n)$ was fitted by application of the harmonic inversion technique to the functional form of the semiclassical trace formula

$$\varrho(w)=\sum_k A_k e^{-2\pi i\tilde{S}_k w}, \tag{10}$$

with complex parameters $A_k$ and $\tilde{S}_k$. For isolated returning orbits these parameters, obtained from the quantum spectra, can directly be compared to the periodic orbit parameters of the classical calculations [19]. The part of the complex action plane which is of interest for the hyperbolic umbilic catastrophe discussed above is presented in Fig. 4. The two solid peaks mark the positions $\tilde{S}_k$ and the absolute values of amplitudes $|A_k|$ obtained from the quantum spectrum. However, there is only one classical ghost orbit which is of physical relevance (dash-dotted peak in Fig. 4). The position of that peak is in good agreement with the quantum result, but the amplitude is enhanced, as is expected for isolated periodic orbit contributions near bifurcations (see Fig. 3). For comparison, we have analyzed the uniform approximation (9) at constant scaled energy $\tilde{E}=-0.1$ and in the same range $0<w<140$, by applying the harmonic inversion technique of Ref. [19]. The results for the uniform approximation are presented as dashed peaks in Fig. 4. The two peaks agree well with the quantum results for both the complex actions and amplitudes. The enhancement of the ghost orbit peak and the

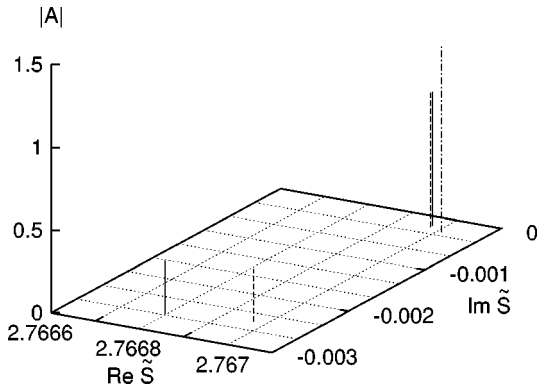


FIG. 4. High resolution recurrence spectra at scaled energy $\tilde{E}=-0.1$. Solid peaks: Part of the quantum recurrence spectra. Dash-dotted peak: Classical ghost orbit contribution. Dashed peaks: Uniform approximation for the hyperbolic umbilic catastrophe.

additional nonclassical peak observed in the quantum spectrum are therefore clearly identified as artifacts of the bifurcation, i.e., the hyperbolic umbilic catastrophe.

In conclusion, we have presented a simple method to construct uniform approximations for the semiclassical density of states, and to relate the parameters of catastrophe diffraction integrals directly to periodic orbit parameters such as classical action and eigenvalues of the stability matrix at energies near the bifurcation. The method is a shortcut to the conventional procedure, i.e., it circumvents the analysis of classical dynamics in the neighborhood of periodic orbits by numerical application of normal form theory, and therefore allows an easy handling of ungeneric bifurcations of several orbits related to catastrophes of higher codimension and corank. This has been demonstrated, by way of example, for a hyperbolic umbilic catastrophe in the diamagnetic Kepler problem, but evidently the method may be applied to other systems and catastrophe types as well. The technique will be useful for a semiclassical quantization of systems with mixed regular-chaotic classical dynamics, e.g., in combination with the method of harmonic inversion which has been successfully applied to systems with complete hyperbolic dynamics [20].

We acknowledge stimulating discussions with F. Haake, H. Schomerus, and T. Uzer, and thank K. Wilmesmeyer for assistance with the classical calculations. This work was supported by the Deutsche Forschungsgemeinschaft (Sonderforschungsbereich No. 237).

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