uniform
approximation
bifurcation!catastrophe
catastrophe

Chapter 44

Uniform approximations

(D. Lippolis)

So far, in dealing with chaotic systems we have always tacitly assumed that all periodic orbits are unstable and isolated. That is true in some open systems, such as scattering off 3 disks in a plane, but any physically interesting bound Hamiltonian system tends to have mixed phase space. In such systems a small parameter change can drive many periodic orbits (of a period shorter than some cutoff) through bifurcations, with orbits arbitrarily close to one another as they collide. Physical parameters, such as slow change of external electric or magnetic fields in atomic and solid state experiments play role of such bifurcation parameters, so study of such bifurcations cannot be avoided. As the classical orbits collide, the corresponding saddlepoints coalesce, and the quadratic, Gaussian stationary phase approximation (33.15) that leads to the Van Vleck propagator (34.30) and the Gutzwiller trace formula (36.3) fails. At the bifurcation point the Jacobian in (36.11) has unit eigenvalues, so the contribution of such periodic orbits to the Gutzwiller trace formula diverges. In this chapter we go beyond the Gaussian saddlepoint approximation, replacing it by approximations uniform in $\hbar$ and parameter/parameters a which describe/describes the distance to the nearest bifurcation.

44.1 Bifurcations and catastrophes

The method of stationary phase can be applied to an integral of the form

☞ sect. 33.2

$$I = \int A(x) \exp\left(is\Phi(x)\right) dx \tag{44.1}$$

by approximating the integrand

$$\Phi(x) \simeq \Phi(x_0) + \frac{1}{2}\Phi''(x_0)\delta x^2 \qquad A(x) \simeq A(x_0) \tag{44.2}$$

normal form
fold catastrophe
catastrophe!fold
cusp catastrophe
catastrophe!cusp

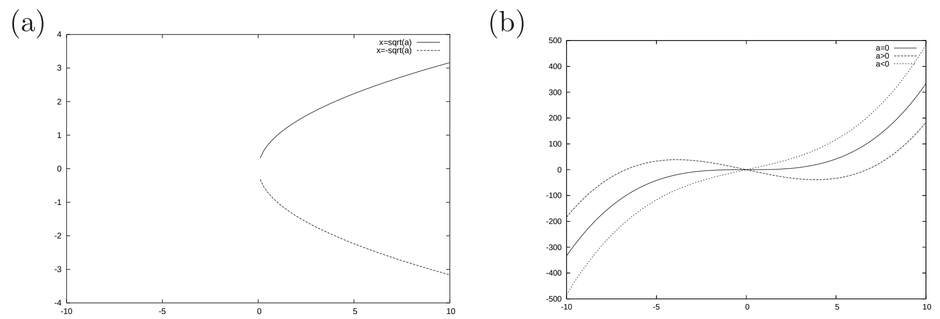


Figure 44.1: Stationary points of (a) the fold catastrophe and (b) the normal form (44.3) for different values of the parameter a.

give an estimate of "sufficiently" far

in the neighborhood of the extremal point (stationary phase point) x_0. When the extremal points are not sufficiently far apart from one another, this approximation fails. Usually the "action" $\Phi(x)$ depends on one or more parameters, with the extremal points getting arbitrarily close to one another and eventually coalescing as the parameters vary. In the neighborhood of the bifurcation parameter values, the function is not well described by the quadratic approximation (44.2). The number of extremal points and their motion as a function of the parameters depends on the local symmetries of the bifurcation. The most robust bifurcation are of codimension one - variation of a single parameter suffices to drive the system through a bifurcation.

Example 44.1 Tangent, pitchfork bifurcation. *Consider the tangent bifurcation plotted in figure 44.1 whose normal form*

$$\Phi_a(x) \simeq \frac{1}{3}x^3 - ax\,, \tag{44.3}$$

is called fold catastrophe. *If the symmetry of the neighborhood of the bifurcation point is such that local map depends on even powers of x^2, the simplest bifurcation is the pitchfork bifurcation plotted in figure 44.2 whose normal form*

$$\Phi_a(x) \simeq \frac{1}{4}x^4 - \frac{1}{2}ax^2\,, \tag{44.4}$$

explain symmetry that forces cusp catstrph

is called cusp catastrophe.

What matters is that while the integral (44.1) can no longer be approximated by a Gaussian integral, it can still can be expressed in terms of special functions.

found many typos, please recheck this part

Example 44.2 Fold, cusp catastrophe. *If the local "action" $\Phi_a(x)$ starts with x^3, then in the neighborhood of the tangent bifurcation a slowly varying amplitude $A_a(x)$ can be approximated by a polynomial of first degree,*

$$\begin{aligned} I &= \int dx\, p(x) e^{i(x^3/3-ax)} = (p_0 + ip_1\, d/da) Ai(a) \\ A_a(x) &\simeq p(x) = p_0 + p_1 x\,, \end{aligned} \tag{44.5}$$

diffraction

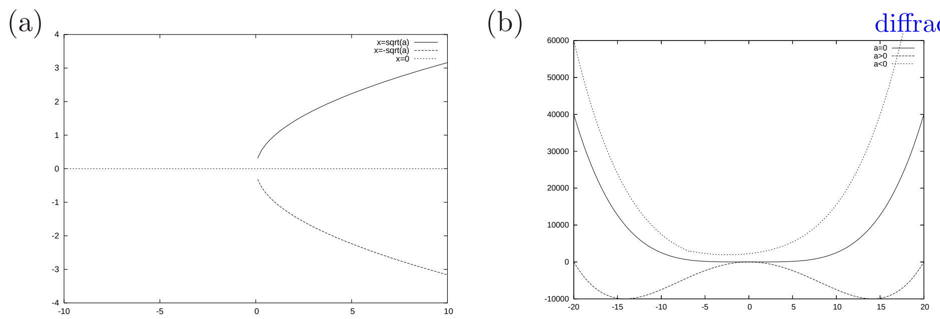


Figure 44.2: Stationary points of (a) the fold catastrophe and (b) the normal form (44.4) for different values of the parameter a.

where

$$Ai(a) = \int dx\, e^{i(x^3/3-ax)} \tag{44.6}$$

is the Airy function. In the case of a cusp catastrophe, the normal form approximation to I requires $A_a(x) \simeq p(x) = p_0 + p_2 x^2$,

$$\begin{aligned} I &\simeq \int dx\, p(x) e^{i(x^4/4-ax^2/2)} = \left(p_0 + 2ip_2 \frac{d}{da}\right) I(a) \\ I(a) &= \int dx\, e^{i(x^4/4-ax^2/2)}\,, \end{aligned} \tag{44.7}$$

where the integral $I(a)$ can be expressed in terms of Bessel functions, [44.9]

no lit refs in the text, → remarks

$$I(a) = \frac{\pi|a|^{\frac{1}{2}}}{2} e^{-i(a^2-\pi)/8} \left(J_{-\frac{1}{4}}(a^2/8) + \mathsf{sign}(a) e^{-i\pi/4} J_{-\frac{1}{4}}(a^2/8)\right)\,. \tag{44.8}$$

formula wrong, fix Bessel indices

insert student HH Roux here

Of course, for simple examples such as a tangent or a pitchfork bifurcation no fancy theory of normal forms and catastrophes is needed, and you might wonder why are worrying about what happens at isolated points (measure zero!) in the classical state space? Doesn't $\hbar$ granularity of the quantum state space take care of that? Well, no. What happens in wave mechanics at manifolds of lower dimensionality is *diffraction*, the quintessentially wave-mechanical phenomenon important when diffracting singularities are of size comparable to the wavelength under study.

Our first example of diffraction, the turning point singularity in the 1-d WKB quantization of sect. 33.4 could be talked away with a bit of Fresnel/Maslov voodoo, so we did not even invoke the word "diffraction". In chapter 42 we saw that when the wavelength is comparable to the size of obstacles, diffraction significantly modifies and extends the original Gutzwiller theory. Similarly, in the scattering of wedges of chapter 43 diffraction became very important, because without it there would be no chaotic dynamics whatsoever.

⇓PRIVATE

⇑PRIVATE

Why should diffraction effects play a physically significant role here, where most of the state space is fraught with unstable periodic orbits, the potential is assumed smooth, and the diffraction is localized to a few orbits? Physical reason is that while individual strongly unstable orbits orbits contribute exponentially small terms to periodic orbits trace sums, marginally stable (intermittent) orbits are on the way to turning into elliptic islands, and their neighborhoods are disproportionally small. That is why, when you look at the bottom of a swimming pool, the main thing that you see is the web by caustics, even though such catastrophes are of much lower dimensionality than the full space.

44.2 Periodic orbits near bifurcations

Since the Gutzwiller trace formula derivation of sect. 36.1 no longer applies, let us start from the beginning: we would like to evaluate the right-hand side of (32.20) the quantum density of states in terms of the trace of the quantum Green's function, that is

$$\begin{aligned} d(E) &= \sum_n \delta(E-E_n) = -\lim_{\epsilon\to 0}\frac{1}{\pi}\mathrm{Im}\,\mathrm{tr}\,G(q,q',E+i\epsilon) \\ &= -\frac{1}{\pi}\mathrm{Im}\int d^2q d^2q' \delta(q-q')\,G(q,q',E) \end{aligned} \qquad (44.9)$$

And here comes the first idea. In a codimension-one bifurcation embedded in a chaotic sea, almost all periodic orbit are unstable and isolated - at any given bifurcation parameter value, a set of only two or three periodic orbits are wed into the bifurcation. So we assume that the VanVleck semiclassical propagator (34.46) is good for q, q' separated by a small distance

$$G(q,q',E) = \frac{1}{i\hbar(2\pi\hbar)^{(D-1)/2}}\frac{1}{|\dot q \dot q'|^{1/2}}\left|\det D_\perp\right|^{1/2} e^{\frac{i}{\hbar}S-\frac{i\pi}{2}m}, \qquad (44.10)$$

We have already evaluated an integral like this in sect. 36.1, and determined that the stationary phase condition enforces that the orbit is not only *closed orbit* returning in the spatial coordinate, but that it is *periodic* in the full state space.

In order to evaluate this in the neighborhood of a bifurcation we have to be bit more careful. While for isolated unstable orbit a Gaussian integral leads to the Gutzwiller trace formula, here we need to write the local action as the appropriate catastrophe normal form, such as the fold (44.3) or cusp (44.4) catastrophe.

And now the second idea: in the neighborhood of a codimension-one bifurcation, we can chose a natural Poincaré section such that the catastrophe dynamics occurs along one $[q,p]$ symplectic plane, and the rest is amenable to the usual Gaussian saddle-point analysis. More formally: the *splitting lemma* of catastrophe theory states that, given a function $f(x_1,...,x_n)$, whose Hessian has rank $n-m$, a coordinate system $q_1, ..., q_n$ can be introduced in the neighborhood of a fixed point, such that

define somewhere Hessian

$$f(q_1, ..., q_n) = g(q_1, ..., q_m) + h(q_{m+1}, ..., q_n)$$

where g has a extremal point degenerate at the origin and h is a non-degenerate quadratic form. In general, the number of parameters that participate in the bifurcation is called codimension of the bifurcation. The examples given in the previous section describe two different codimension-one bifurcations, since there is only one parameter – a – to tune. The splitting lemma tells us that the action (i.e., function f) can be split into a catastrophe polynomial plus a nondegenerate function that can hence be integrated with the saddle point approximation.

Example 44.3 2-dof system. *Let us show what happens in the simple case of a 2-dimensional system. First of all we choose a local frame of reference in the phase space with one coordinate along the orbit (called z) and the other one (y) perpendicular to it. The action is initially defined as a function of y, y', z, z', however, the Poincaré map (as well as the fundamental matrix matrix) is close to the identity near a bifurcation, so that it cannot be generated by a function of the initial and final coordinates ($y = y'$!). For this reason it is necessary to use a mixed coordinate-momentum representation of the action, by applying a Legendre transform*

$$S(z', y'z, y, E) = \tilde{S}(z', y', z, p_y, E) - yp_y$$

at the same time we replace one of the delta functions in (44.10) by

$$\delta(y - y') = \frac{1}{2\pi\hbar}\int dp_y e^{\frac{i}{\hbar}p_y(y-y')}\,.$$

That is because the function $\tilde{S}(p_y, y') - y'p_y$ is stationary at every fixed point of the Poincaré section defined by $z = const.$ and $E = const.$ The integral (44.10) is now proportional to

$$\int_{z'=z+l} dzdy'dp_y \|\det D\|^{1/2} \exp\left(\frac{i}{\hbar}\hat{S}(z', y', z, p_y, E) - \frac{i}{\hbar}y'p_y - \frac{i\pi}{2}m\right) \tag{44.11}$$

where l is the length of the orbit. Finally, we switch to normal coordinates on the Poincaré section so that $\hat{S} = \hat{S}(p, q', E)$ at $z' = z + l$. The transformation produces a factor of $1/\dot{z}$ in the integral (44.11), that now reads

$$\int_0^l \frac{dz}{\dot{z}} \int dq'dp \left\|\frac{\partial\hat{S}}{\partial p\partial q'}\right\|^{1/2} \exp\left(\frac{i}{\hbar}\hat{S}(q', p, E) - \frac{i}{\hbar}q'p - \frac{i\pi}{2}m\right). \tag{44.12}$$

The first integral is just the period of the orbit. In the vicinity of the bifurcation, the action $S(q', p, E)$ can be expanded as a normal form. For simple examples such as a tangent or a pitchfork bifurcation no theory of normal forms is needed. It is enough to recall that a fixed point of the Poincaré map is a stationary point of the function $\hat{S}(q', p) - q'p$ in order to guess that a tangent bifurcation will yield

$$\hat{S}(q', p, E) = S_0(E) + q'p - \frac{1}{2}p^2 - aq' - q'^3$$

closed orbit

and a pitchfork bifurcation will give

$$\hat{S}(q', p, E) = S_0(E) + q'p - \frac{1}{2}p^2 - aq'^2 - q'^4 .$$

no lit refs in the text, → remarks

S_0 and a can be expressed in terms of the actions and amplitudes of the orbits involved in the bifurcation [44.5], so that the integrals (44.12) are now easy. The one over p is a Gaussian integral, while the one over q' can be expressed in terms of Airy or Bessel functions. More precisely, the determinant $|\det D|^{1/2}$ brings a polynomial of the first order in q', so that the whole integral can still be expressed in terms of the Airy function plus its first derivative with respect to the parameter a. Note that there exists a neighborhood $\Delta a \simeq \hbar$ around the bifurcation, necessitating inclusion of ghost orbits in the expansion, for the parameter values for which they participate in the bifurcation.

explain ghost orbits

44.1
page 830

44.3 Closed orbits

like having closed orbits here - another example of diffraction!

Closed orbit theory is used to study interactions of atoms with external static fields semiclassically. When an atom absorbs a photon, the electron goes into an outgoing Coulomb wave, which propagates away from the nucleus, until the wave fronts can be correlated with outgoing classical trajectories. Eventually the wave fronts are scattered back by the (electro)magnetic field, and interfere with the outgoing waves to produce the observed oscillations in the average-absorption spectrum. It turns out that the main contributions to the oscillating spectrum are given by the classical trajectories which start and end close to the nucleus, i.e. the closed orbits. Spectroscopic measurements do not give the density of states, but rather the oscillator strengths, defined as

$$f_n = 2(E_n - E_i)|\langle i|D|n\rangle|^2 , \tag{44.13}$$

where D is the component of the dipole operator describing the polarization of the exciting electromagnetic field. The density of oscillator strength

$$f(E) = \sum_n f_n \delta(E - E_n) \tag{44.14}$$

(and hence every single strength) can conveniently be expressed in terms of the quantum mechanical response function

$$g(E) = -\frac{1}{\pi}\sum_n \frac{|\langle i|D|n\rangle|^2}{E - E_n + i\epsilon} = -\frac{1}{\pi}\langle i|DG(E)D|i\rangle \tag{44.15}$$

by the relation

$$f(E) = 2(E - E_i)\,\mathrm{Im}\,[g(E)] . \tag{44.16}$$

It is possible to compute $g(E)$ semiclassically, by using the Van Vleck approximation to the retarded Green's function $G(E)$. The result has the same form as the Gutzwiller trace formula:

Closed orbit!bifurcation

$$g(E) = g_0(E) + g^{osc}(E)$$

where g_0 is a smooth contribution independent of the interaction with the external fields and

$$g^{osc}(E) = \sum_{co} \mathcal{A}_{co}(E) e^{i(S_{co}(E) - \frac{\pi}{2}\mu_{co})}\,, \tag{44.17}$$

is given as a sum over all the classical closed orbits. In the expression above, S_{co} is the action of the closed orbit, μ_{co} its topological index and

$$\mathcal{A}_{co} = 4\pi \frac{\mathcal{Y}^*(\theta_f, \phi_f)\mathcal{Y}(\theta_i, \phi_i)}{\sqrt{|M|}} \tag{44.18}$$

is a function of the initial and final angles (the $\mathcal{Y}$'s are linear combinations of spherical harmonics that characterize the initial or the final state) and

$$M = (\sin(\theta_i)\sin(\theta_f))^{-1} \det \frac{\partial(p_{\theta_f}, p_{\phi_f})}{\partial(\theta_i, \phi_i)} \tag{44.19}$$

is the ratio between the determinant of the fundamental matrix and the symmetric matrix of second derivatives of the action (that arises from the stationary phase approximation).

44.3.1 Closed orbits near bifurcations

The main point is that M vanishes at a bifurcation, that is why we need uniform approximations.

To that end, one starts with the results of the previous section for periodic orbits, and obtaines similar expressions in the case of bifurcations of closed orbits, by taking a reasonable ansatz for the uniform approximation of contribution to the response function

$$\Psi(E) = I(a) e^{iS_0(E)} \tag{44.20}$$

where

$$I(a) = \int dx\, p(x) e^{i\Phi_a(x)}\,. \tag{44.21}$$

Here $p(x)$ and $S_0(E)$ are unknown, while $\Phi_a(x)$ is a suitable normal form for the bifurcation in question, which we again assume to only depend on one parameter. The strategy is now to evaluate the unknowns from the limit of (44.20) far away from the bifurcation, where (44.21) can be computed by means of the stationary phase approximation to yield

$$\Psi(E) = \sum_{x_i} \frac{(2\pi i)^{1/2} p(x_i)}{\sqrt{|Hess \Phi_a(x_i)|}} \exp\left[i(S_0(E) + \Phi_a(x_i) - \pi\nu_i/2)\right], \quad (44.22)$$

where ν_i is the number of negative eigenvalues of the Hessian (5.9) and the sum is over all the extremal points x_i of $\Phi_a(x)$. Comparing the latter expression with the general form (44.17) of $\Psi(E)$, we can infer that

$$S_i(E) = S_0(E) + \Phi_a(x_i) \quad (44.23)$$

and hence find the values of $S_0(E)$ and the extremal points of $\Phi_a(x_i)$. As long as we are dealing with real orbits, ν_i corresponds to the topological index, otherwise it has to be determined so that $p(x_i)$ be continuous through the bifurcation [44.9]. However, that is not enough to determine $p(x)$ uniquely. Considering $p(x)$ is needed only in the neighborhood of $x = 0$, it is wise to Taylor-expand it about such point, so as to obtain a polynomial ansatz, with the coefficients to be determined from the values of the semiclassical amplitudes of (44.22) evaluated in the extremal points. Of course all that can be possible only if the polynomial has degree $k-1$, where k is the number of orbits involved in the bifurcation. Everything is best explained by a simple example , such as

no lit refs in the text, → remarks

Example 44.4 Tangent bifurcation/fold catastrophe.

$$\Phi_a(x) = \frac{1}{3}x^3 - ax$$

which has extremal points at $x = \pm\sqrt{a}$, real if $a > 0$, so that

$$\Phi_a(\pm\sqrt{a}) = \mp\frac{2}{3}a^{2/3}$$

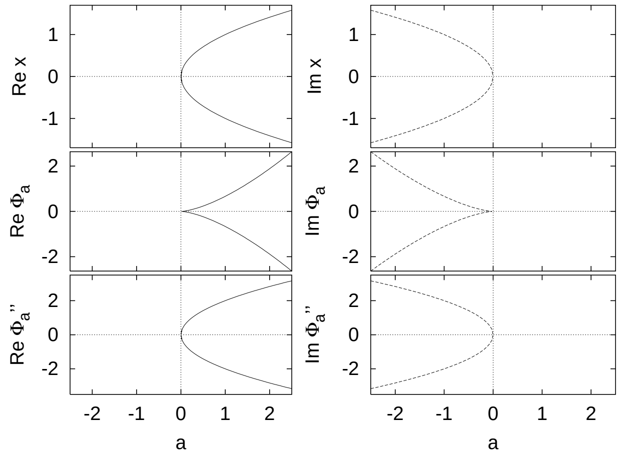
are its stationary values. Figure 44.3 illustrates the positions of extremal points, stationary values and second derivatives in the fold catastrophe. It is evident that both $\Phi_a(x_i)$ and $\Phi_a''(x_i)$ are real even for $a < 0$, when the extremal points x_i's are complex, that is they correspond to ghost orbits having real actions and stability determinants.

Now we can evaluate $S_0(E)$ and a as functions of S_1, S_2, by using (44.23):

$$S_1 = S_0(E) - \frac{2}{3}a^{3/2}, \qquad S_2 = S_0(E) + \frac{2}{3}a^{3/2}$$

that leads to

$$S_0(E) = \frac{1}{2}(S_1 + S_2), \qquad |a| = \left(\frac{3}{4}|S_2 - S_1|\right)^{2/3}.$$



normal form

Figure 44.3: The positions of extremal points, stationary values and second derivatives in the fold catastrophe. Solid lines indicate extremal points, dashed lines complex extremal points. Dotted lines are coordinate axes. (T. Bartsch [44.9])

We also need an expression for the amplitudes, for which it is necessary to determine $p(x)$. *Equation (44.22) yields*

$$\mathcal{A}_1 = \frac{\sqrt{\pi}}{|a|^{1/4}} p(\sqrt{a}) e^{i\pi/4} , \qquad \mathcal{A}_2 = \frac{\sqrt{\pi}}{|a|^{1/4}} p(-\sqrt{a}) e^{-i\pi/4} . \tag{44.24}$$

If $p(x)$ *is a polynomial of the form*

$$p(x) = (p_0 + p_1 x)/2\pi$$

then the parameters p_0 *and* p_1 *read*

$$p_0 = \pi |a|^{1/4} e^{-i\pi/4} (\mathcal{A}_1 + i\mathcal{A}_2) , \qquad p_1 = \pi |a|^{-1/4} e^{-i\pi/4} (\mathcal{A}_1 - i\mathcal{A}_2)$$

so that now everything is known in the formula (44.21), which becomes

$$\int dx \, (p_0 + p_1 x) e^{i\Phi_a(x)}$$

and can be evaluated in terms of the Airy function and its derivative with respect to a

$$\int dx \, e^{i\Phi_a(x)} = Ai(-a) , \qquad \int dx \, x \, e^{i\Phi_a(x)} = -iAi'(-a) ,$$

once S_1, S_2, $\mathcal{A}_1$ *and* $\mathcal{A}_2$ *have been computed, see figure 44.4.*

Commentary

Remark 44.1 Normal forms. The classification of all the possible bifurcation scenarios and corresponding normal forms is the realm of catastrophe theory [44.1], with higher codimension bifurcations requiring simultaneous fine tuning of more parameters and thus being less generic. The theory of normal forms is used to simplify nonlinear systems trough a near-identity change of variables. In the present context, it can be used to expand the action to a polynomial in the vicinity of a bifurcation [44.6].

uniform approximation
symmetry breaking
closed orbit
orbit!closed

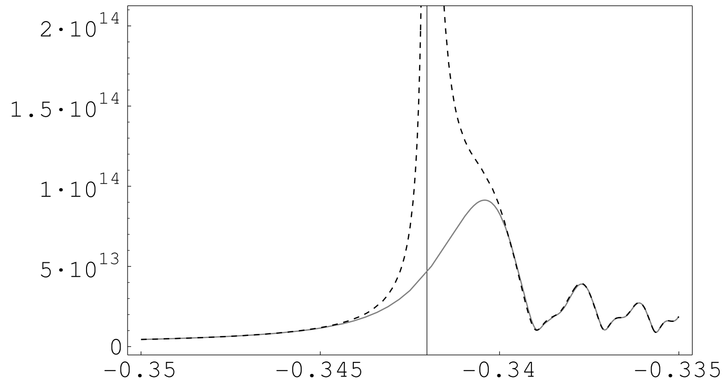


Figure 44.4: Magnitude of the contribution to the response function of the bifurcating orbits plotted versus the scaled energy [44.10]. The Gutzwiller trace formula (44.22) (dashed curve) diverges at the bifurcating point; the uniform approximation (44.20) (solid curve) interpolates smoothly between the values of the Gutzwiller trace formula on either side of the bifurcation.

Remark 44.2 Uniform approximations. Initially designed to include marginally stable orbits in the Gutzwiller trace formula, uniform approximations have found many applications in atomic physics. Work on diffraction integrals containing catastrophes was done in optics by Berry and Upstill [44.2]. Ozorio de Almeida and Hannay [44.3] and Schomerus and Sieber [44.5, 44.4] have developed uniform approximations near bifurcations of periodic orbits. Uniform approximations in closed orbit theory have been addressed by Gao and Delos [44.13] and Shaw and Robicheaux [44.12] for an atom in an electric field, and by Main and Wunner [44.11] and Bartsch [44.9] in for an atom in crossed electric and magnetic fields. When the change of a continous parameter causes the breaking of a symmetry of the system, a number of degenerate orbits may suddenly disappear. Uniform approximations for such bifurcations can be found in Creagh [44.14] and Brack *et al.* [44.15].

Remark 44.3 Closed orbits. Closed orbit theory was formulated in 1988 by Du, Delos [44.7] and Bogomolny [44.8], in order to explain the existence of oscillations in the average-absorption spectrum of an atom in a magnetic field.

give references: hydrogen in crossed electric and magnetic fields, if useful

Résumé

The method of (Gaussian) stationary phase approximation fails whenever two or more extremal points of the approximated function are too close to one another. In such cases higher order terms in expansion of classical action need to be kept, leading to uniform approximations in terms of functions of Airy or Bessel type that enables a smooth interpolation of trace formulas through bifurcation values. Coalescence of saddles occurs at bifurcation values of parameters of the classical dynamics. For periodic orbits close to bifurcations the Gutzwiller trace formula diverges, and the action needs to be expanded according to catastrophe/normal form theory. The method applies to bifurcations of closed orbits as well, since the contributions to the spectral density of the colliding orbits ultimately depend on their amplitudes and actions only.

not sure this explains it

References

[44.1] T. Poston and I. Stewart, *Catastrophe Theory and its applications* (Dover, 1996).

[44.2] M.V. Berry and C. Upstill, *Prog. in Optics* **18**, 257 (1980).

[44.3] A.M. Ozorio de Almeida and J.H. Hannay, *J. Phys. A* **20**,5873 (1987).

[44.4] M. Sieber, *J. Phys. A* **29**, 4715 (1996).

[44.5] H. Schomerus and M. Sieber, *J. Phys. A* **30**, 4537 (1997).

[44.6] P. Leboeuf and A. Mouchet, "Normal forms and complex periodic orbits in semiclassical expansions of Hamiltonian systems", *Ann. Phys.* **275**, 54 (1999); `chao-dyn/9809015`.

[44.7] M.L. Du and J.B. Delos, *Phys. Rev. A* **38**, 1896 (1988).

[44.8] E.B. Bogomolny, *Sov. Phys. JETP* **69**, 265 (1989).

[44.9] T. Bartsch, *The hydrogen atom in an electric field and in crossed electric and magnetic fields: Closed-orbit theory and semiclassical quantization*, Ph. D. thesis (Cuvillier Verlag, Göttingen 2002).

[44.10] T. Bartsch, J. Main, and G. Wunner, *Prog. Theor. Phys. Suppl.* **139**, 429 (2000).

[44.11] J. Main and G. Wunner, *Phys. Rev. A* **55**, 1743 (1997).

[44.12] J.A. Shaw and F. Robicheaux, *Phys. Rev. A* **58**, 1910 (1998).

[44.13] J. Gao and J.B. Delos, *Phys. Rev. A* **56**, 356 (1997).

[44.14] S.C. Creagh, *Ann. Phys.* **248**, 60 (1996).

[44.15] M. Brack *et al.*, *JPA* **32**, 331 (1999).