PHYSICS ON AND NEAR CAUSTICS

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Février 1997

IHES/M/97/22

PHYSICS ON AND NEAR CAUSTICS

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Abstract

Physics *on* caustics is obtained by studying physics *near* caustics. Physics on caustics is at the cross-roads of calculus of variation and functional integration. More precisely consider a space $\mathcal{PM}^d$ of paths $x : [t_a, t_b] \rightarrow \mathbf{M}^d$, on a d -dimensional manifold $\mathbf{M}^d$. Consider two of its subspaces:

i) The $2d$ -dimensional space $\mathcal{U}$ of critical points of an action functional $S : \mathcal{PM}^d \rightarrow \mathbf{R}$; $q \in \mathcal{U} \Leftrightarrow \frac{\delta S}{\delta q} = 0$.

ii) The space $\mathcal{P}_{\mu, \nu} \mathbf{M}^d$ of paths satisfying d initial conditions (μ) and d final conditions (ν).

The nature of the intersection $\mathcal{P}_{\mu, \nu} \mathbf{M}^d \cap \mathcal{U}$ is the key to identifying and analyzing caustics. Caustics occur when the roots of $S'(q) = 0$, for S restricted to $\mathcal{P}_{\mu, \nu} \mathbf{M}^d$, are not isolated points in $\mathcal{U}$. We consider two cases:

i) The roots define a subspace of non zero dimension ℓ of $\mathcal{U}$. For example, the classical system with action S is constrained by conservation laws.

ii) There is a multiple root of $S'(q) = 0$. For example the classical flow has an envelope.

In both situations there is, at least, one nonzero Jacobi field along q with d initial vanishing boundary conditions (μ) and d final vanishing boundary conditions (ν), i.e. $q(t_a)$ and $q(t_b)$ are conjugate points along q . In both cases we say " $q(t_b)$ is on the caustics".

The strict WKB approximations of functional integrals for the system S "break down" on caustics, but the full semiclassical expansion, including contributions from $S''(q)$ and $S'''(q)$ (and possibly higher derivatives) yield the physical properties of the system S on and near the caustics. Caustics display classical physics as a limit of quantum mechanics.

We work out glory scattering cross-sections because, there, both situations occur simultaneously: the system is constrained by conservation laws, and the classical flow is caustic forming. The cross-section is given in closed form in section V.

I. Introduction

Interesting phenomena occur when a flow of classical paths is caustic forming. Glory scattering, rainbows, orbiting, etc... are only a few examples of physics on and near caustics. Conservation laws are, as we shall see, another example.

Physics on caustics is at the cross-roads of calculus of variation and functional integration. More precisely consider a space $\mathcal{P}\mathbf{M}^d$ of $(L^{2,1})$ paths

$$x : \mathbf{T} \rightarrow \mathbf{M}^d \quad , \quad \mathbf{T} = [t_a, t_b]$$

on a d -dimensional manifold $\mathbf{M}^d$. Consider two of its subspaces:

i) the $2d$ -dimensional subspace $\mathcal{U}$ of critical points of an action functional

$$(I.1) \quad S : \mathcal{P}\mathbf{M}^d \rightarrow \mathbb{R}$$

$$(I.2) \quad q \in \mathcal{U} \Leftrightarrow \frac{\delta S}{\delta q} = 0;$$

ii) the space $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$ of paths satisfying d boundary conditions (μ) at $t = t_a$, and d boundary conditions (ν) at $t = t_b$.

The nature of the intersection

$$(I.3) \quad \mathcal{U}_{\mu,\nu} := \mathcal{P}_{\mu,\nu} \mathbf{M}^d \cap \mathcal{U}$$

is the key to identifying and analyzing caustics.

Fig. 1. $\mathcal{U}$ is the space of classical motions (critical points of the action functional S); $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$ is the space of paths satisfying d initial conditions and d final conditions; $\mathcal{U}_{\mu,\nu}$ is their intersection.

In the context of functional integration, the action functional S is restricted to $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$; unless otherwise specified we assume here S to be restricted to $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$. Caustics can be analyzed by studying the expansion of S around $S(q)$ with $q \in \mathcal{U}_{\mu,\nu}$, namely

$$(I.4) \quad S(x) = S(q) + S'(q) \cdot \xi + \frac{1}{2!} S''(q) \cdot \xi\xi + \frac{1}{3!} S'''(q) \cdot \xi\xi\xi + \dots$$

$$(I.5) \quad x = q + \xi$$

where ξ has d vanishing boundary conditions at t_a , and d vanishing boundary conditions at t_b . For q in $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$ we have

$$(I.6) \quad q \in \mathcal{U}_{\mu,\nu} \Leftrightarrow S'(q) \cdot \xi = 0 \text{ for all } \xi \text{ in } T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d.$$

We can consider 4 cases:

- i) $\mathcal{U}_{\mu,\nu}$ consists of isolated points: no caustics, e.g. the anharmonic oscillator (provided (μ, ν) does not define a conjugate point).
- ii) $\mathcal{U}_{\mu,\nu}$ is a space of dimension $\ell > 0$: conservation laws.
- iii) $q \in \mathcal{U}_{\mu,\nu}$ is a multiple root: the classical flow has an envelope.
- iv) $\mathcal{U}_{\mu,\nu}$ is an empty set.

In case i) the critical points are not degenerate; in cases ii) and iii) the critical points are degenerate.

In case i) we need to keep only the second variation.

In case ii) we need to keep also the first variation.

In case iii) we need to keep (at least) the first three variations.

In this paper, we shall not consider the case in which $\mathcal{U}_{\mu,\nu}$ is an empty set; this case is interesting but does not belong to the study of caustics. A typical example is the knife edge problem solved by L.S. Schulman [1 and references therein].

There is another wording to distinguish cases ii) and iii) from case i): “The WKB approximation of the functional integral for the transition $K(\nu, t_b; \mu, t_a)$ of the system governed by S breaks down in cases ii) and iii)”.

These different wordings reflect the different ways one approaches the intersection $\mathcal{U}_{\mu,\nu}$, namely from $\mathcal{U}$ (calculus of variation) or from $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$ (functional integration). They are equivalent because an eigenvector of the Jacobi operator with zero eigenvalue is also a nonzero Jacobi field with vanishing boundary conditions at t_a and t_b .

II. Degenerate critical points

Fixing the boundary conditions (μ) and (ν) , the point q in $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$ is said to be a *critical point of S* if

$$(II.1) \quad S'(q) \cdot \xi = 0 \text{ for all } \xi \text{ in } T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d.$$

It is said to be degenerate if the hessian form of S is degenerate; this condition means that, for some $\eta \neq 0$ in $T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d$, one has

$$(II.2) \quad S''(q) \cdot \xi \eta = 0 \text{ for all } \xi \text{ in } T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d.$$

The integral kernel of the hessian is the (functional) Jacobi operator

$$(II.3) \quad \mathcal{J}_{\alpha\beta}(q, s, t) = \frac{1}{2} \frac{\delta^2}{\delta \xi^\alpha(s) \delta \xi^\beta(t)} S''(q) \cdot \xi \xi.$$

The hessian defines the (differential) Jacobi operator on $T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d$ by

$$(II.4) \quad S''(q) \cdot \xi \xi = \langle \xi, \mathcal{J}(q) \xi \rangle = \int_{\mathbf{T}} dt \xi^\alpha(t) \mathcal{J}_{\alpha\beta}(q(t)) \xi^\beta(t).$$

Here ξ is a $L^{2,1}$ vector field along q and $\langle \cdot, \cdot \rangle$ is the $L^{2,1}$ duality. See in the Appendix the explicit expression for $S''(q) \cdot \xi \xi$ when S is not restricted to $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$. It is useful when one explores $\mathcal{U}_{\mu,\nu}$ by varying the (μ) and/or the (ν) boundary conditions.

A *Jacobi field* $h(q)$ is a vector field along q in the space $T_q \mathcal{U}$; it is obtained by a variation through classical paths around q . It is therefore a solution of the Jacobi equation

$$(II.5) \quad \mathcal{J}_{\alpha\beta}(q(t)) h^\beta(q(t)) = 0 \quad h \in T_q \mathcal{U}$$

often abbreviated to

$$\mathcal{J}_{\alpha\beta}(q) h^\beta(t) = 0.$$

To say that the hessian is degenerate is to say that there is at least one nonzero Jacobi field $h \in T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d$, that is at least one nonzero Jacobi field with d vanishing boundary conditions at t_a and d at t_b . Equivalently, the hessian is degenerate if the Jacobi operator has one or more eigenvectors in $T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d$ with zero eigenvalue.

The eigenvectors of the Jacobi operator form a convenient basis of $T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d$ because they diagonalize the hessian, and the hessian is the best quadratic form for defining a volume element on $T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d$. Explicitly let $\{\psi_k\}$ be a complete set of orthonormal eigenvectors of the Jacobi operator in the space $T_q \mathcal{P}_{\mu,\nu} \mathbf{M}^d$:

$$(II.6) \quad \mathcal{J}(q) \psi_k(t) = \alpha_k \psi_k(t) \quad k \in \{0, 1, \dots\}.$$

There may be ℓ zero eigenvalues,

$$\alpha_k = 0 \quad k \in \{0, \dots, \ell - 1\};$$

$$(II.7) \quad \int_{\mathbf{T}} dt (\psi_k(t) | \psi_j(t)) = \delta_{kj}.$$

We expand ξ in this basis

$$(II.8) \quad \xi^\alpha(t) = \sum_{k=0}^{\infty} u^k \psi_k^\alpha(t)$$

$$(II.9) \quad S''(q) \cdot \xi \xi = \langle \xi, \mathcal{J}(q) \xi \rangle = \sum_{k=0}^{\infty} \alpha_k (u^k)^2 = \sum_{k=\ell}^{\infty} \alpha_k (u^k)^2.$$

We call $\ell^2(\text{hessian})$ the space of points u such that $\sum \alpha_k (u^k)^2 < \infty$. On the subspace $\mathbf{X} \subset T_q \mathcal{P}_{\mu, \nu} \mathbf{M}^d$ spanned by the eigenvectors $\{\psi_k\}$ with nonzero eigenvalues, $S''(q) \cdot \xi \xi$ defines a nondegenerate quadratic form $Q(u)$

$$(II.10) \quad Q(u) := S''(q) \cdot \xi \xi |_{\mathbf{X}} = \sum_{k=\ell}^{\infty} \alpha_k (u^k)^2$$

$\mathbf{X}$ is parametrized by $\{u^k\}$ for $k \in \{\ell, \dots\}$.

With ξ expanded in the eigenvector basis $\{\psi_k\}$, the first, second, and third variations of $S(x)$ around $S(q)$ read

$$(II.11) \quad \begin{aligned} S'(q) \cdot \xi &= \int_{\mathbf{T}} dt \frac{\delta S}{\delta q^\alpha(t)} \sum_{k=0}^{\infty} u^k \psi_k^\alpha(t) \\ &= \sum_{k=0}^{\infty} \left(\int_{\mathbf{T}} dt \frac{\delta S}{\delta q^\alpha(t)} \psi_k^\alpha(t) \right) u^k =: \sum_{k=0}^{\infty} c_k u^k \end{aligned}$$

$$(II.12) \quad S''(q) \cdot \xi \xi = \sum_{k=0}^{\infty} \alpha_k (u^k)^2, \text{ with } \alpha_k \text{ the eigenvalues of (II.6)}$$

$$(II.13) \quad S'''(q) \cdot \xi \xi \xi = \sum_{k, \ell, m} \left(\int_{\mathbf{T}} dr \int_{\mathbf{T}} ds \int_{\mathbf{T}} dt \frac{\delta^3 S}{\delta q^\alpha(r) \delta q^\beta(s) \delta q^\gamma(t)} \psi_k^\alpha(r) \psi_\ell^\beta(s) \psi_m^\gamma(t) \right) \cdot u^k u^\ell u^m.$$

For k between 0 and $\ell - 1$, ψ_k is a Jacobi field with d vanishing boundary conditions at t_a and d vanishing boundary conditions at t_b .

Explicit calculations of an eigenvector of the Jacobi operator with zero eigenvalue.

Jacobi fields, with or without vanishing boundary conditions, are derivatives of one parameter families of classical solutions. For instance let $q \in \mathcal{U}$ be specified by its *initial* position and *initial* momentum

$$(II.14) \quad q(t_a, a, p_a) = a, \quad p(t_a, a, p_a) = p_a$$

then the set of $2d$ Jacobi fields

$$(II.15) \quad \begin{cases} \partial q^\alpha(t, a, p_a) / \partial p_{a\beta} =: j^{\alpha(\beta)}(t) \\ \partial q^\alpha(t, a, p_a) / \partial a^\beta =: k_{(\beta)}^\alpha(t) \end{cases}$$

is a particularly useful basis for $T_q \mathcal{U}$. Also useful in phase space, and in the study of caustics is the set

$$(II.16) \quad \begin{cases} \partial p_\alpha(t, a, p_a) / \partial p_{a\beta} =: \tilde{k}_\alpha^{(\beta)}(t) \\ \partial p_\alpha(t, a, p_a) / \partial a^\beta =: \ell_{\alpha(\beta)}(t) \end{cases}$$

$\tilde{k}^{(\beta)}$ and $\ell_{(\beta)}$ are not Jacobi fields in configuration space but the matrices $J, K, \tilde{K}, L$, whose columns consist of the components of $j^{(\beta)}, k_{(\beta)}, \tilde{k}^{(\beta)}, \ell_{(\beta)}$ respectively,

$$(II.17) \quad J^{\alpha\beta}(t, t_a) = j^{\alpha(\beta)}(t)$$

$$(II.18) \quad K_\beta^\alpha(t, t_a) = k_{(\beta)}^\alpha(t)$$

$$(II.19) \quad \tilde{K}_\alpha^\beta(t, t_a) = \tilde{k}_\alpha^{(\beta)}(t)$$

$$(II.20) \quad L_{\alpha\beta}(t, t_a) = \ell_{\alpha(\beta)}(t),$$

together make a $2d \times 2d$ matrix $\mathbf{J}$ of Jacobi fields in phase space, namely;

$$(II.21) \quad \mathbf{J}(t, t_a) := \begin{pmatrix} J^{\alpha\beta}(t, t_a) & K_\beta^\alpha(t, t_a) \\ \tilde{K}_\alpha^\beta(t, t_a) & L_{\alpha\beta}(t, t_a) \end{pmatrix}.$$

Therefore we call $J, K, \tilde{K}, L$ “Jacobi matrices”. The properties of the Jacobi matrices are simple and powerful tools for solving problems [2-5]. Here we shall use them to express a Jacobi field ψ_0 with vanishing boundary conditions:

$$(II.22) \quad \text{If } \psi_0(t_a) = 0, \text{ then } \psi_0(t) = J(t, t_a) \dot{\psi}_0(t_a).$$

$$(II.23) \quad \text{If } \dot{\psi}_0(t_a) = 0, \text{ then } \psi_0(t) = K(t, t_a) \psi_0(t_a).$$

$$(II.24) \quad \text{If } \dot{\psi}_0(t_b) = 0, \text{ then } \psi_0(t) = \psi_0(t_b) \tilde{K}(t_b, t).$$

The case of derivatives vanishing both at t_a and t_b is best discussed in phase space path integrals (see reference [6] and [4]). To prove (II.22, 23, 24), note that both sides of the equations satisfy the same differential equation and the same boundary values at t_a (for eq. II.22, 23) or at t_b (for eq. II.24).

To construct a Jacobi field ψ_0 such that $\psi_0(t_a) = 0$ and $\psi_0(t_b) = 0$, it suffices therefore by (II.22) to choose $\dot{\psi}_0(t_a)$ in the kernel of the linear map $J(t_b, t_a)$. A similar procedure applies for the two other cases $\dot{\psi}_0(t_a) = 0, \psi_0(t_b) = 0$ in (II.23) and $\psi_0(t_a) = 0, \dot{\psi}_0(t_b) = 0$ in (II.24).

III. The intersection $\mathcal{U}_{\mu, \nu}$ is of dimension $\ell > 0$; constants of the motion

This situation has a finite-dimensional analog when S is a function, rather than a functional, namely the critical points of S are not isolated and Morse's lemma needs to be generalized.

1. Generalized Morse lemma; finite dimensional case

Let $S : \mathbf{M}^d \rightarrow \mathbb{R}$ be a smooth function on a d -dimensional manifold $\mathbf{M}^d$. Its Taylor expansion around a point x_0 reads

$$(III.1) \quad S(x) = S(x_0) + S'_\alpha(x_0) y^\alpha + \frac{1}{2} S''_{\alpha\beta}(x_0) y^\alpha y^\beta + O(|y|^3)$$

with coordinates y^α vanishing at x_0 . We consider the case in which there exists a submanifold $\mathbf{V}^\ell \subset \mathbf{M}^d$ of dimension ℓ , such that

$$(III.2) \quad T_{x_0} \mathbf{M}^d = T_{x_0} \mathbf{V}^\ell \oplus T_{x_0} \mathbf{F}^{d-\ell}$$

for some supplementary manifold $\mathbf{F}^{d-\ell}$ of dimension $d - \ell$ through x_0 . We assume that $S'(x_0)$ induces 0 on $T_{x_0} \mathbf{F}^{d-\ell}$ but that the hessian

$$(III.3) \quad S''(x_0) \text{ is not degenerate on } T_{x_0} \mathbf{F}^{d-\ell},$$

and induces 0 on $T_{x_0} \mathbf{V}^\ell$.

Possibly after a linear change of coordinates, we shall have two sets of equations

$$(III.4) \quad \begin{cases} S'_a = g_a & \text{constant on } \mathbf{V}^\ell; \\ S'_A(x_0) = 0 & \text{determine } d - \ell \text{ coordinates of } x_0. \end{cases}$$

In physical terms, the first set of equations corresponds to a constrained system, or to conservation laws. The second set of equations defines a *relative critical point*, under the constraints $S'_a(x_0) = g_a$. In the new coordinates, labelled y^a and y^A , with $1 \leq a \leq \ell$, $\ell + 1 \leq A \leq d$, one gets

$$(III.5) \quad S(x) = S(x_0) + g_a y^a + \frac{1}{2} S''_{AB}(x_0) y^A y^B + O(|y|^3).$$

A non linear change of the variables $\{y^A\} \mapsto \{\bar{y}^A\}$ can now be used to remove the terms of order greater than 2, according to the Morse lemma.

We express the situation in more geometrical terms. The space $\mathbf{M}^d$ is fibered by $(d - \ell)$ -dimensional fibres $\mathbf{F}^{d-\ell}(g_a)$; each fibre is defined by the values of $\{g_a\}$. On each fibre there is a non degenerate critical point. Such critical points will be said to be *relative to a given fibre* because we take the variations of S along the fibers. The set of relative critical points define a (in general local) section of the fibered space $\mathbf{M}^d$.

Fig. 2. The space $\mathbf{M}^2$ is fibered by the fibres $\mathbf{F}(g)$. The function S restricted to $\mathbf{F}(g)$ has a nondegenerate relative critical point.

In conclusion, if the (relative) first variation $S'(x_0) = 0$ defines a submanifold $\mathbf{V}^\ell$, and if the second variation S'' restricted to the complement of $\mathbf{V}^\ell$ in $\mathbf{M}^d$ is not degenerate, the generalized Morse lemma says that there exists a system of coordinates $(\bar{y}^a, \bar{y}^A)$ in the neighborhood of a relative critical point x_0 such that

$$(III.6) \quad S(x) = S(x_0) + \sum_{a=1}^{\ell} g_a \bar{y}^a + \sum_{A,B=\ell+1}^d g_{AB}(x_0) \bar{y}^A \bar{y}^B.$$

Remark. The extreme cases $\ell = 0$ (isolated critical points) and $\ell = d$ (no critical point) are well known.

2. Generalized Morse lemma; infinite dimensional case; Lagrange multipliers

Equation (I.4) is the infinite dimensional version of (III.1). Formally the argument leading from (III.1) to the generalized Morse lemma (III.6) applies to (I.4). But the contents is much richer in the infinite dimensional case:

- the algebraic equations for the critical points $x_0 \in \mathbf{M}^d$ become equations for q in $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$, i.e. Euler-Lagrange differential equations.
- The set of Euler-Lagrange equations splits into 2 sets:

$$(III.7) \quad \begin{cases} S'_a = g_a & \text{is a set of } \ell \text{ constraints on the system} \\ S'_A(q) = 0 & \text{determine the components } q^A \text{ of the path } q : T \rightarrow \mathbf{M}^d. \end{cases}$$

Equation (III.5) now reads, with the notation of section I

$$(III.8) \quad S(x) = S(q) + g_a \cdot \xi^a + \frac{1}{2} S''_{AB}(q) \cdot \xi^A \xi^B + O(|\xi|^3).$$

The variables $\{\xi^a\}$ play the role of Lagrange multipliers of the system.

In a functional integral symbolically written

$$(III.9) \quad \int_{\Xi} \exp(2\pi i S(x)/h) \mathcal{D}_{\Xi} \xi$$

with

$$(III.10) \quad \mathcal{D}_{\Xi} \xi = \mathcal{D}\xi^a \mathcal{D}\xi^A$$

the integration with respect to $\mathcal{D}\xi^a$ contributes δ -functionals in g_a . In equation (III.23) we shall give explicitly the linear change of variables, $\xi \mapsto u$, which brings the action in the form (III.5). We do not have a general prescription for the non linear change of variable which would remove $O(|\xi|^3)$.

Remark. The nonlinear change of variable $x \mapsto z$, exploited in [8], which brings the second variation into a quadratic form on $\mathcal{P}\mathbb{R}^d$ is valid only on spaces of pointed paths. It can be used here if we replace $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$ by a space of pointed paths, say $\mathcal{P}_{\mu} \mathbf{M}^d$, and insert in the integrand an index function which kills the paths which are not in $\mathcal{P}_{\mu,\nu} \mathbf{M}^d$.

Remark. The generalized Morse lemma in finite dimensions was derived in [3]; it was used for the infinite dimensional case by constructing the WKB approximation of a propagator when the final state is restricted by a conservation law. For example, with obvious notations, one writes, K being the WKB approximation of the propagator,

$$K(p_b, t_b; p_a, t_a) = \lim_{h=0} \int_{\mathbf{M}^d} dx K(p_b, t_b; x, t) K(x, t; p_a, t_a)$$

and looks for the critical points of the sum $F(x)$ of the action functions $\mathcal{S}$ (not the action functionals S)

$$F(x) = \mathcal{S}(p_b, t_b; x, t) + \mathcal{S}(x, t; p_a, t_a).$$

The analysis of the degenerate critical points of the function $F(x)$ reproduces the results obtained in Section III.1, and Section III.2. If $F(x)$ has no critical point, i.e. if there is no classical path between (p_a, t_a) and (p_b, t_b) , then $K(p_b, t_b; p_a, t_a) = O(\hbar^n)$ for n an arbitrary integer. It follows that *conservation laws* (here conservation of momentum) *appear only in the classical limit of quantum physics*.

3. Functional integral; semiclassical approximation

The functional integral representation of the probability amplitude $K(\nu, t_b; \mu, t_a)$ for the transition of the system S from the state μ at t_a to the state ν at t_b can be written schematically

$$(III.11) \quad K(\nu, t_b; \mu, t_a) = \int_{\mathcal{P}_{\mu, \nu} \mathbf{M}^d} \mathcal{D}x \exp \left(\frac{2\pi i}{\hbar} S(x) \right) \Phi(x(t_a)).$$

The domain of integration $\mathbf{X}$ is the space of $L^{2,1}$ paths

$$x : \mathbf{T} \rightarrow \mathbf{M}^d$$

satisfying boundary conditions (μ) at t_a , and (ν) at t_b .

The semiclassical approximation is a path integral over the tangent space $T_q \mathcal{P}_{\mu, \nu} \mathbf{M}^d$. To fit within the general framework of [8], we recall the expressions as written there for semiclassical approximations when the second variation is not degenerate. We recall a specific case: “momentum-to-position” transition [8, §III.2], because it is more illuminating than a generic case. One of the important points of [8] is to integrate over a space of pointed paths (paths with one fixed point) because a space of pointed paths on any manifold $\mathbf{M}^d$ is contractible and can be parametrized by a space of pointed paths on $\mathbb{R}^d$, vanishing at the origin of $\mathbb{R}^d$. In a momentum-to-position transition, the obvious parametrizing space is the space $\mathcal{P}_0 T_b \mathbf{M}^d$ of paths on $T_b \mathbf{M}^d$ where $x(t_b) = b$.

The (ν) boundary conditions are $x(t_b) = b$.

The (μ) boundary conditions at t_a are encoded in the functional integral by the choice of initial “wave function” Φ in (III.11) – a plane wave of momentum $p(t_a) = p_a$ if $\mathbf{M}^d$ is flat, or its “generalization” [8, eq. (III.2)] if $\mathbf{M}^d$ is riemannian.

If the hessian of S is not degenerate, the strict WKB approximation [8, eq. III.17] of $K(b, t_b; p_a, t_a)$ is [9]

$$(III.12) \quad K_{\text{WKB}}(b, t_b; p_a, t_a) = \exp \left(\frac{2\pi i}{\hbar} \mathcal{S}(t_b, x_b) \right) \left(\text{Det} \frac{Q_0}{Q + Q_0} \right)^{1/2}$$

where $\mathcal{S}$ is the action function, solution of the Hamilton-Jacobi equation of the system and where by [8, eq. (B.30)]

$$(III.13) \quad Q_0(\xi) + Q(\xi) = \frac{2}{h} S''(q) \cdot \xi \xi$$

with

$$Q_0(\xi) = \int_{\mathbf{T}} dt \frac{\partial^2 L}{\partial \dot{q}^\alpha(t) \partial \dot{q}^\beta(t)} \dot{\xi}^\alpha(t) \dot{\xi}^\beta(t).$$

The infinite determinant in (III.12) is the ratio of finite determinants of Jacobi matrices (see [8, section III.2] [10 and references therein]. The determinant in (III.12) together with (III.13) comes from [8, eq. (B.34)]

$$(III.14) \quad \int \mathcal{D}_{s, Q_0} \xi \exp \left(-\frac{2\pi}{sh} S''(q) \cdot \xi \xi \right) = \left(\text{Det} \frac{Q_0}{Q_0 + Q} \right)^{1/2}, \quad s \in \{1, i\}.$$

This equation can be thought of as defining $\mathcal{D}_{s, Q_0}$ on $T_q \mathcal{P}_{\mu, \nu} \mathbf{M}^d$. Anticipating the case in which the hessian of S is degenerate, we make the linear change of variable defined by (II.8)

$$(III.15) \quad L : T_q \mathcal{P}_{\mu, \nu} \mathbf{M}^d \rightarrow \ell^2(\text{hessian}) \text{ by } \xi \mapsto u$$

with $\ell^2(\text{hessian})$ the space of points u such that $\sum \alpha_k (u^k)^2$ is finite (see II.9). Moreover, assume for simplicity that there is only one eigenvector ψ_0 of the Jacobi operator which has a zero eigenvalue.

We recall briefly the transformation of a functional integral under a linear change of variable of integration [see 8, §A2.2]. Let

$$L : \mathbf{X} \rightarrow \mathbf{Y},$$

let $\mathcal{D}x$ on $\mathbf{X}$ be defined by

$$(III.16) \quad \int_{\mathbf{X}} \mathcal{D}x \exp \left(-\frac{\pi}{s} Q_{\mathbf{X}}(x) - 2\pi i \langle x', x \rangle \right) = \exp(-\pi s W_{\mathbf{X}'}(x'))$$

$Q_{\mathbf{X}}$ a quadratic form on $\mathbf{X}$, $W_{\mathbf{X}'}$ its “inverse” in the dual $\mathbf{X}'$ of $\mathbf{X}$, whose precise definition [8, (I.6)] is not needed here. Let $\mathcal{D}y$ on $\mathbf{Y}$ be defined similarly by

$$(III.17) \quad \int_{\mathbf{Y}} \mathcal{D}y \exp \left(-\frac{\pi}{s} Q_{\mathbf{Y}}(y) - 2\pi i \langle y', y \rangle \right) = \exp(-\pi s W_{\mathbf{Y}'}(y'))$$

where, assuming L invertible

$$(III.18) \quad Q_{\mathbf{Y}} = Q_{\mathbf{X}} \circ L^{-1}, \text{ i.e. } Q_{\mathbf{Y}}(y) = Q_{\mathbf{X}}(x(y)).$$

Then,

$$(III.19) \quad \int_{\mathbf{X}} \mathcal{D}x \exp \left(-\frac{\pi}{s} Q_{\mathbf{X}}(x) \right) \cdot g(Lx) = \int_{\mathbf{Y}} \mathcal{D}y \exp \left(-\frac{\pi}{s} Q_{\mathbf{Y}}(y) \right) \cdot g(y).$$

Therefore, (III.14) in the u variable reads

$$(III.20) \quad \begin{aligned} \int_{T_q \mathcal{P}_{\mu, \nu} \mathbf{M}^d} \mathcal{D}_{s, Q_0} \xi \exp \left(-\frac{\pi}{s} Q_0(\xi) \right) \exp \left(-\frac{\pi}{s} Q(\xi) \right) \\ = \int \mathcal{D}_{s, Q_0 \circ L^{-1}} u \exp \left(-\frac{\pi}{s} Q_0(\xi(u)) \right) \exp \left(-\frac{\pi}{s} Q(\xi(u)) \right) \\ = \int \mathcal{D}_{s, Q_0 \circ L^{-1}} u \exp \left(-\frac{2\pi}{sh} S''(q) \cdot \xi(u) \xi(u) \right). \end{aligned}$$

The domain of integration $\ell^2(\text{hessian})$ is spanned by the complete set of eigenvectors $\{\psi_k\}$, $k \in \{0, \dots\}$, and can be decomposed into a one-dimensional space $\mathbf{X}^1$ spanned by ψ_0 and an infinite dimensional space $\mathbf{X}^\infty$ of codimension 1, spanned by $\{\psi_k\}$, $k \in \{1, \dots\}$

$$(III.21) \quad \ell^2(\text{hessian}) = \mathbf{X}^1 \times \mathbf{X}^\infty.$$

The volume element on $\ell^2(\text{hessian})$ is the product of the volume elements on $\mathbf{X}^1$ and on $\mathbf{X}^\infty$ respectively. We write

$$(III.22) \quad \mathcal{D}_{s, Q_0 \circ L^{-1}} u = \mathcal{D}_{\mathbf{X}^1} u^0 \mathcal{D}_{\mathbf{X}^\infty} u.$$

Under the change (III.15) defined by (II.8), the dominating terms in the expansion of $S(x)$ around $S(q)$ read (III.8)

$$(III.23) \quad S(x) \simeq S(q) + c_0 u^0 + \frac{1}{2} \sum_{k=1}^{\infty} \alpha_k (u^k)^2$$

with

$$(III.24) \quad c_0 = \int_{\mathbf{T}} dt \frac{\delta S}{\delta q^\alpha(t)} \psi_0^\alpha(t)$$

and the functional integral, with $s = i$,

$$(III.25) \quad \begin{aligned} \int \mathcal{D}_{i, Q_0 \circ L^{-1}} u \exp \left(\frac{2\pi i}{h} c_0 u^0 + \frac{\pi i}{h} \sum_{k=1}^{\infty} \alpha_k (u^k)^2 \right) \cdot \Phi(x(t_a)) \\ = \int_{\mathbf{X}^1} \mathcal{D}_{\mathbf{X}^1} u^0 \exp \left(\frac{2\pi i}{h} c_0 u^0 \right) \int_{\mathbf{X}^\infty} \mathcal{D}_{\mathbf{X}^\infty} u \exp \left(\frac{\pi i}{h} \sum_{k=1}^{\infty} \alpha_k (u^k)^2 \right) \cdot \Phi(x(t_a)). \end{aligned}$$

In the space $\mathbf{X}^\infty$, the quadratic form

$$S''(q) \cdot \xi \xi |_{\mathbf{X}^\infty} = \sum_{k=1}^{\infty} \alpha_k (u^k)^2$$

is invertible and the integral over $\mathbf{X}^\infty$ proceeds as before. The integral over $\mathbf{X}^1$ contributes a δ -function to the propagator

$$\delta \left(\frac{1}{h} \int_{\mathbf{T}} dt \frac{\delta S}{\delta q^\alpha(t)} \psi_0^\alpha(t) \right)$$

which says that the propagator vanishes, unless the conservation law

$$\frac{1}{h} \int_{\mathbf{T}} dt \frac{\delta S}{\delta q^\alpha(t)} \psi_0^\alpha(t) = 0$$

is satisfied.

Explicit expressions for a variety of cases can be found in [3]. In conclusion, if the action is invariant under automorphisms of $\mathcal{U}_{\mu,\nu}$, then the dominating terms of the semi-classical expansion of $S(x)$ around $S(q)$ imply conservation laws. Conservation laws appear in the classical limit of quantum physics.

IV. The intersection $\mathcal{U}_{\mu,\nu}$ is a multiple root of $S'(q) \cdot \xi = 0$

In this situation the classical flows are caustic forming. Four examples are treated in references [11] and [4]. Two of them enter into well-known problems.

i) The soap bubble problem [12]. The “paths” are the curves defining (by rotation around an axis) the surface of a soap bubble held by two rings. The “classical flow” is a

family of catenaries with one fixed point. The caustic is the envelope of the catenaries.

Fig. 3. For a point in the “dark” side of the caustic there is no classical path; for a point on the “bright” side there are two classical paths which coalesce into a single one as the intersection of the two paths approaches the caustic. Note that the paths do not arrive at an intersection at the same time, the paths do not intersect in a space time diagram.

ii) The scattering of particles by a repulsive Coulomb potential. The flow is a family of Coulomb paths with fixed initial momentum. Its envelope is a parabola.

Fig. 4. A flow on configuration space of charged particles in a repulsive Coulomb potential.

The two other examples are not readily identified as caustic problems because the

flows do not have an envelope in the physical space. The vanishing boundary conditions of the Jacobi field at the caustic is the vanishing of its first derivative. In phase space the projection of the flow on the momentum space has an envelope.

- iii) Rainbow scattering from a point source.
- iv) Rainbow scattering from a source at infinity.

The relevant features can be analyzed on a specific example. We choose the scattering of particles by a repulsive Coulomb potential since we have already discussed momentum-to-position transitions in Section III. For other examples see [7].

Let q and q^Δ be two solutions of the same Euler-Lagrange equation with slightly different boundary conditions at t_b

$$\begin{aligned} p(t_a) &= p_a & q(t_b) &= b \\ p^\Delta(t_a) &= p_a & q^\Delta(t_b) &= b^\Delta. \end{aligned}$$

Assume p_a and b to be conjugate along q with multiplicity 1; i.e. the Jacobi fields h along q such that

$$\dot{h}(t_a) = 0, \quad h(t_b) = 0$$

form a one-dimensional space. Assume (p_a, b^Δ) not conjugate along q^Δ .

We shall compute the probability amplitude $K(b^\Delta, t_b; p_a, t_a)$ when b^Δ is close to the caustic on the “bright” side or on the “dark” side. We shall *not* compute K by expanding S around q^Δ for the following reasons:

- If b^Δ is on the dark side, q^Δ does not exist.
- If b^Δ is on the bright side, one could consider K to be the limit of the sum of two contributions corresponding to the two paths q and q^Δ intersecting at b^Δ

$$K(b, t_b; p_a, t_a) = \lim_{\Delta=0} K_q(b^\Delta, t_b + \Delta t; p_a, t_a) + K_{q^\Delta}(b^\Delta, t_b; p_a, t_a)$$

but, at b^Δ , q has touched the caustic and “picked up” an additional phase equal to $-\pi/2$; both limits are infinite and their sum is not defined.

We compute $K(b^\Delta, t_b; p_a, t_a)$ by expanding S around q , using (I.4) – and possibly higher derivatives if the third variation is singular. The calculation requires some care [see reference [7] for details] because $q(t_b) \neq b^\Delta$; in other words q is not a critical point of the action restricted to the space of paths such that $x(t_b) = b^\Delta$.

As before we make the change (II.8) of variable $\xi \mapsto u$ which diagonalizes $S''(q) \cdot \xi \xi$. In the u variable, the expansion of $S(x)$ is given by (II.11, 12, 13). Again we decompose the domain of integration in the u -variable

$$\ell^2(\text{hessian}) = \mathbf{X}^1 \times \mathbf{X}^\infty.$$

Again the second variation restricted to $\mathbf{X}^\infty$ is non singular, and calculating the integral over $\mathbf{X}^\infty$ proceeds as usual for the strict WKB approximation. The integral over $\mathbf{X}^1$ is

$$(IV.1) \quad I(\nu, c) = \int_{\mathbf{R}} du^0 \exp \left(i \left(cu^0 - \frac{\nu}{3} (u^0)^3 \right) \right) = \nu^{-1/3} \text{Ai}(\nu^{-1/3} c)$$

where

$$(IV.2) \quad \nu = \frac{\pi}{h} \int_{\mathbf{T}} dr \int_{\mathbf{T}} ds \int_{\mathbf{T}} dt \frac{\delta^3 S}{\delta q^\alpha(r) \delta q^\beta(s) \delta q^\gamma(t)} \psi_0^\alpha(r) \psi_0^\beta(s) \psi_0^\gamma(t)$$

$$(IV.3) \quad c = -\frac{2\pi}{h} \int_{\mathbf{T}} dt \frac{\delta S}{\delta q(t)} \cdot \psi_0(t) (b^\Delta - b)$$

Ai is the Airy function. The leading contribution of the Airy function when h tends to zero can be computed by the stationary phase method. At $v^2 = \nu^{-1/3} c$

$$(IV.4) \quad \text{Ai}(\nu^{-1/3} c) \simeq \begin{cases} 2\sqrt{\pi} v^{-1/4} \cos\left(\frac{2}{3} v^2 - \frac{\pi}{4}\right) & \text{for } v > 0 \\ \sqrt{\pi} (-v)^{-1/4} \exp\left(-\frac{2}{3} v^3\right) & \text{for } v < 0 \end{cases}$$

v is the critical point of the phase in the integrand of the Airy function; it is of order $h^{-1/3}$. For $v > 0$, b^Δ is in the illuminated region and the probability amplitude oscillates rapidly as h tends to zero. For $v < 0$, b^Δ is in the shadow region and the probability amplitude decays exponentially.

The probability amplitude $K(b^\Delta, t_b; a, t_a)$ does not blow up when b^Δ tends to b . Quantum mechanics softens up the caustics.

Remark. The normalization and the argument of the Airy function can be expressed solely in terms of the Jacobi fields.

Remark. Other cases, such as position-to-momentum, position-to-position, momentum-to-momentum, angular momentum transitions have been treated explicitly in references [3] and [7].

V. Glory scattering

Backward scattering of light, very close to the direction of the incoming rays has a long and interesting history (see for instance [13] and references therein). It creates a bright halo around one's shadow, and is usually called glory scattering. Early derivations of glory scattering were cumbersome, and used several approximations. It has been computed from

first principles by functional integration using only the expansion in powers of the square root of Planck's constant [11,4].

The classical cross-section for the scattering of a beam of particles in a solid angle $d\Omega = 2\pi \sin \theta d\theta$ by an axisymmetric potential is

$$(V.1) \quad d\sigma_{cl}(\Omega) = 2\pi B(\theta) dB(\theta)$$

where the deflection function $\Theta(B)$ giving the scattering angle θ as a function of the impact parameter B is assumed to have a unique inverse $B(\Theta)$. We can write

$$(V.2) \quad d\sigma_{cl}(\Omega) = B(\Theta) \frac{dB(\Theta)}{d\Theta} \Big|_{\Theta=\theta} \frac{d\Omega}{\sin \theta}$$

abbreviated henceforth

$$(V.3) \quad d\sigma_{cl}(\Omega) = B(\theta) \frac{dB(\theta)}{d\theta} \frac{d\Omega}{\sin \theta}.$$

It can happen that for a certain value of B , say B_g (g for glory), the deflection function vanishes,

$$(V.4) \quad \theta = \Theta(B_g) \text{ is } 0 \text{ or } \pi,$$

implying $\sin \theta = 0$, and making (V.3) useless.

The classical glory scattering cross-section is infinite because glory scattering is a caustic problem on two accounts.

i) There is a conservation law: the final momentum $p_b = -p_a$ the initial momentum.

ii) Near glory, particles with impact parameter $B_g + \delta B$ and $-B_g + \delta B$ exist with approximately the same angles, namely $\pi +$ terms of order $(\delta B)^3$.

The glory cross-section can be computed [11,4] using the methods presented in sections III and IV. The result is

$$(V.5) \quad d\sigma(\Omega) = 4\pi^2 h^{-1} |p_a| B^2(\theta) \frac{dB(\theta)}{d\theta} J_0(2\pi h^{-1} |p_a| B(\theta) \sin \theta)^2 d\Omega$$

where J_0 is the Bessel function of order 0.

A similar calculation [14,4,13] gives the WKB cross-section for polarized glories of massless waves in curved spacetimes

$$(V.6) \quad d\sigma(\Omega) = 4\pi^2 \lambda^{-1} B_g^2 \frac{dB}{d\theta} J_{2s}(2\pi \lambda^{-1} B_g \sin \theta)^2 d\Omega$$

$s = 0$ for scalar waves; at glory $J_0(0)^2 \neq 0$

$s = 1$ for electromagnetic waves; at glory $J_2(0)^2 \neq 0$

$s = 2$ for gravitational waves; at glory $J_4(0)^2 \neq 0$.

λ is the wave length of the incoming wave.

Equation (V.6) matches perfectly with the numerical calculations [13] of R. Matzner based on the partial wave decomposition method.

Fig. 5. Glory Cross-Section

$$\frac{d\sigma}{d\Omega} = 2\pi\omega B_g^2 \left| \frac{dB}{d\theta} \right|_{\theta=\pi} J_{2s}(\omega B_g \sin \theta)^2$$

$B_g = B(\pi)$ glory impact parameter

$\omega = 2\pi\lambda^{-1}$; $s = 2$ for gravitational wave

analytic cross section: dashed line

numerical cross section: solid line

VI. Conclusion

Caustics are classical limits of quantum physics. They are best characterized by the existence of nonvanishing Jacobi fields with vanishing boundary conditions. They include conservation laws as well as caustics in the strict sense of the term.

Appendix

Although it is often easier to work with eq. II.4 rather than with the differential form of the Jacobi operator obtained via integration by parts, we record the differential form below, not assuming vanishing boundary conditions for ξ at t_a nor at t_b . This equation can be useful in particular when varying the boundary conditions.

Let $S(q) = \int_T dt L(q(t), \dot{q}(t), t)$; then, the Jacobi operator defined by

$$S''(q) \cdot \xi \xi = \int_T dt \xi^\alpha(t) \mathcal{J}_{\alpha\beta}(q(t)) \xi^\beta(t) + \Sigma(t_b) - \Sigma(t_a)$$

can be written (abbreviating $q(t)$ by q and $\xi(t)$ by ξ)

$$\mathcal{J}_{\alpha\beta}(q) = -\frac{\partial^2 L}{\partial \dot{q}^\alpha \partial \dot{q}^\beta} \frac{d^2}{dt^2} + \left(\frac{\partial^2 L}{\partial q^\alpha \partial \dot{q}^\beta} - \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial q^\beta} - \frac{d}{dt} \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial \dot{q}^\beta} \right) \frac{d}{dt} - \frac{d}{dt} \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial q^\beta} + \frac{\partial^2 L}{\partial q^\alpha \partial q^\beta}$$

and the boundary terms

$$\Sigma(\cdot) = \left(\frac{\partial^2 L}{\partial \dot{q}^\alpha \partial q^\beta} - \frac{1}{2} \frac{d}{dt} \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial \dot{q}^\beta} \right) \xi^\alpha \xi^\beta + \frac{1}{2} \frac{d}{dt} \left(\frac{\partial^2 L}{\partial \dot{q}^\alpha \partial \dot{q}^\beta} \xi^\alpha \xi^\beta \right),$$

equivalently

$$\Sigma(t) = \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial q^\beta} \xi^\alpha \xi^\beta + \frac{\partial^2 L}{\partial \dot{q}^\alpha \partial \dot{q}^\beta} \dot{\xi}^\alpha \xi^\beta.$$

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