5

Semiclassical Expansion; Beyond WKB

5.1 Introduction

When "WKB breaks down ..." then rainbows and glory scattering may appear. In other words, and with the notation of chapter 4, when the hessian $S''(q)$ of the functional S is degenerate

$$S''(q) \cdot \xi\xi = 0 \tag{5.1}$$

for $q \in \mathcal{J}_{\mu,\nu}\, \mathbb{M}^D$, $\xi \in T_q \mathcal{J}_{\mu,\nu} \mathbb{M}^D$, $\xi \neq 0$, there is at least one nonzero Jacobi field h along q

$$S''(q)h = 0, \quad h \in T_q U^{2D} \tag{5.2}$$

with D vanishing initial conditions $\{\mu\}$ and D vanishing final conditions $\{\nu\}$. This sentence is the theme which will be developed in chapter 5.

Fig. 5.1.

Notation:

$\mathcal{P}M\!\!\!I^D$: space of paths $x : T\!\!\!T \to M\!\!\!I^D$, $T\!\!\!T = \{t_a, t_b\}$

$\mathcal{P}_{\mu,\nu}M\!\!\!I^D$: space of paths with D boundary conditions $\{\mu\}$ at t_a and D boundary conditions $\{\nu\}$ at t_b

$U^{2D}(s)$: space of critical points of S (a.k.a. solutions of the Euler-Lagrange equation $S'(q)\xi = 0$)

$$U_{\mu,\nu} := U^{2D} \cap \mathcal{P}_{\mu,\nu}M\!\!\!I^D \tag{5.3}$$

In the previous chapter, the intersection $U_{\mu,\nu}$ consists of only one point q, or several isolated points. In section 5.2 entitled "Constants of motion", the action functional is invariant under automorphisms of the intersection $U_{\mu,\nu}$. The intersection is of dimension $\ell > 0$. In section 5.3 entitled "Caustics" the classical flow has an envelope. The intersection $U_{\mu,\nu}$ is the multiple root of $S'(q) = 0$. Glory scattering (section 5.4) is an example where both kinds of degeneracies, conservation law and caustics, occur together. In section 5.5 entitled "Tunneling", the intersection $U_{\mu,\nu}$ is an empty set.

Degenerescence in finite dimensions

The finite dimensional case can be used as an example for classifying the various types of degeneracy of $S''(q) \cdot \xi\xi$.

$$\text{Let } S : \ \mathbf{R}^2 \to \mathbf{R}, \ x = (x^1, x^2) \in I\!\!R^2.$$

Example 1: $S(x) = x^1 + (x^2)^2$; relative critical points. (See section 5.2.) The first derivatives, $\frac{\partial S}{\partial x^1} = 1$ and $\frac{\partial S}{\partial x^2} = 2x^2$; there is no critical point x_0 such that $S'(x_0) = 0$; however, on any subspace $x^1 =$ constant, $x^2 = 0$ is a critical point. We say that $x^2 = 0$ is a relative critical point (relative to the subspace $x^1 =$ constant).

$$\begin{gathered} S''(x) = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} a^1 \\ a^2 \end{pmatrix} = \begin{pmatrix} 0 \\ 2a^2 \end{pmatrix} \\ S''(x)_{ij} a^i b^j = 0 \text{ for all } b \text{ when } a = \begin{pmatrix} a^1 \\ 0 \end{pmatrix} \neq 0. \end{gathered} \tag{5.4}$$

$S''(x)$ is degenerate.

Example 2: $S(x) = (x^2)^2 + (x^1)^3$; double roots of $S'(x_0) = 0$. (See section 5.3.)

$$S'(x_0) = 0 \quad \Rightarrow \quad (x_0^1)^2 = 0,\ x_0^2 = 0$$

$$S''(x) = \begin{pmatrix} 6x^1 & 0 \\ 0 & 2 \end{pmatrix},\ S''(x_0) = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix} \tag{5.5}$$

$S''(x)$ is not degenerate, but $S''(x_0)$ is degenerate at the critical point. In this case we can say the critical point x_0 is degenerate.

The tangent spaces at the intersection

The intersection $U_{\mu,\nu}$ is analyzed in terms of the tangent space at q to $P_{\mu,\nu}M^D$ and U^{2D}.

(i) *A basis for* $T_q\mathcal{P}_{\mu,\nu}M^D$, $q \in U^{2D}$, $S\colon \mathcal{P}_{\mu,\nu}M^D \to \mathbf{R}$.
Consider the restriction of the action functional S to $\mathcal{P}_{\mu,\nu}M$ and expand $S(x)$ around $S(q)$.

$$S(x) = S(q) + S'(q)\cdot\xi + \frac{1}{2!}S''(q)\cdot\xi\xi + \frac{1}{3!}S'''(q)\cdot\xi\xi\xi + \cdots \tag{5.6}$$

The vector field $\xi \in T_q\mathcal{P}_{\mu,\nu}M^D$ has D vanishing boundary conditions at t_a and D vanishing boundary conditions at t_b dictated by the (μ) and (ν) conditions satisfied by all $x \in \mathcal{P}_{\mu,\nu}M^D$. The second variation is the hessian

$$S''(q)\cdot\xi\xi = \langle \mathcal{J}(q)\cdot\xi, \xi\rangle \tag{5.7}$$

where $\mathcal{J}(q)$ is the Jacobi operator on $T_q\mathcal{P}_{\mu,\nu}M^D$. A good basis for $T_q\mathcal{P}_{\mu,\nu}M^D$ diagonalizes the hessian: in its diagonal form the hessian may consist of a finite number of zeroes, say ℓ, and a nondegenerate quadratic form of codimension ℓ. The hessian is diagonalized by the eigenvectors of the Jacobi operator. (Appendix IE eqs. E.45–E.48.) In brief let $\{\Psi_k\}_k$ be a complete set of orthonormal eigenvectors of $\mathcal{J}(q)$:

$$\mathcal{J}(q)\cdot\Psi_k = \alpha_k\Psi_k,\ k \in \{0, 1, \ldots\}. \tag{5.8}$$

Let $\{u^k\}$ be the coordinates of ξ in the $\{\Psi_k\}$ basis

$$\xi^a(t) = \sum_{k=0}^{\infty} u^k\Psi_k^\alpha(t), \tag{5.9}$$

$$u^k = \int_{t_a}^{t_b} dt(\xi(t)|\Psi_k(t)). \quad (5.10)$$

$$S''(q) \cdot \xi\xi = \sum_{k=0}^{\infty} \alpha_k (u^k)^2; \quad (5.11)$$

Therefore the space of the $\{u^k\}$ is the (hessian) space l^2 of points u such that $\sum \alpha_k (u^k)^2$ is finite.

(ii) *A basis for $\mathcal{U}^{\in}$: a complete set of linearly independent Jacobi fields.*
Let h be a Jacobi field, i.e. let h satisfy the Jacobi equation

$$\mathcal{J}(q) \cdot h = 0. \quad (5.12)$$

The Jacobi fields can be obtained without solving this equation: the critical point q is a function of t and of two constants of integration. The two derivatives of q with respect to the constants of integration are Jacobi fields.

If one (or several) eigenvalues of the Jacobi operator vanishes - assume only one, say $\alpha_0 = 0$, for simplicity - then Ψ_0 is a Jacobi field with vanishing boundary conditions

$$\mathcal{J}(q) \cdot \Psi_0 = 0, \;\; \Psi_0 \in T_q\mathcal{P}_{\mu,\nu}M^d. \quad (5.13)$$

The $2D$ Jacobi fields are not linearly independent, $S''(q) \cdot \xi\xi$ is degenerate. When there exists a Jacobi field Ψ_0 along with vanishing boundary conditions, the end points $q(t_a)$ and $q(t_b)$ are said to be conjugates of each other. The above construction of Jacobi fields needs to be modified slightly.

(iii) *Construction of Jacobi fields with vanishing boundary conditions.*
The Jacobi matrices, J, K, $\tilde{K}$, L, defined in Appendix IE (E.18), can be used for constructing Jacobi fields such as $\mathbf{\Psi}_0$ defined by (5.13).

$$\text{If } \Psi_0(t_a) = 0, \quad \text{then} \quad \Psi_0(t) = J(t, t_a)\dot{\Psi}_0(t_a). \quad (5.14)$$
$$\text{If } \dot{\Psi}_0(t_a) = 0, \quad \text{then} \quad \Psi_0(t) = K(t, t_a)\Psi_0(t_a). \quad (5.15)$$
$$\text{If } \dot{\Psi}_0(t_b) = 0, \quad \text{then} \quad \Psi_0(t) = \Psi_0(t_b)\tilde{K}(t_b, t). \quad (5.16)$$

To prove (5.14)–(5.16) note that both sides satisfy the same differential equation and the same boundary conditions at t_a or t_b.

For constructing a Jacobi field such that $\Psi_0(t_a) = 0$ and $\Psi_0(t_b) = 0$, it suffices to choose $\dot{\Psi}_0(t_a)$ in the kernel of $J(t_b, t_a)$. A similar procedure applies to the two other cases. The case of derivatives vanishing both at t_a and t_b is best treated in phase space path integrals [1],[2].

In conclusion, a zero eigenvalue Jacobi eigenvector is a Jacobi field with vanishing boundary condition. Such a Jacobi field creates degenerecence.

5.2 Constants of the motion

The intersection $U_{\mu,\nu} := U^{2D} \cap \mathcal{P}_{\mu,\nu}\mathbb{M}^D$ can be said to be at the crossroad of calculus of variation and functional integration. Coming to the crossroad from functional integration one sees classical physics as a limit of quantum physics. Conservation laws, in particular, emerge at the classical limit.

The Euler-Lagrange equation $S'(q) = 0$ which determine the critical points $q \in U^{2D}_{\mu,\nu}$ consist of D coupled equations

$$S'_\alpha(q) := \delta S(x)/\delta x^\alpha(t)\big|_{x=q} . \tag{5.17}$$

It can happen, possibly after a chage of variable in the space of paths $\mathcal{P}_{\mu,\nu}\mathbb{M}^D$, that this system of equations split into two sets

$$S'_a = g_a \qquad \text{for } a \in \{1, \ldots, \ell\} \quad a \text{ constant} \tag{5.18}$$

$$S'_A(q) = 0 \qquad \text{for } A \in \{\ell + 1, \ldots, D\}. \tag{5.19}$$

The ℓ equations (5.18) are constraints; the $D - \ell$ equations (5.19) determine $D - \ell$ coordinates q^A of q. The space of critical points $U_{\mu,\nu}$ is of dimension ℓ. The second set (5.19) defines a relative critical point under the constraints $S'_a(q) = g_a$. The expansion (5.6) of the action functional now reads

$$S(x) = S(q) + g_a\xi^a + \frac{1}{2}S''_{AB}(q)\xi^A\xi^B + \mathcal{O}\left(|\xi|^3\right). \tag{5.20}$$

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

In a functional integral, symbolically written

$$\int_{\Xi} \{\mathcal{D}\xi^a\} \left\{\mathcal{D}\xi^A\right\} \exp(2\pi\imath S(x)/h) \tag{5.21}$$

the integrations with respect to $\{\mathcal{D}\xi^a\}$ give δ-functions in $\{g_a\}$.

The decomposition $\mathcal{D}\xi$ into $\{\mathcal{D}\xi^a\}\left\{\mathcal{D}\xi^A\right\}$, is conveniently achieved by the linear change of variable of integration (5.9) (5.10)

$$L : T_q\mathcal{T}_{\mu,\nu}\mathbb{M}^D \to \boldsymbol{X} \text{ by } \xi \mapsto u; \tag{5.22}$$

it is not affected by the fact that ℓ eigenvectors $\boldsymbol{\Psi}_k$, $k \in \{0, \ldots, \ell-1\}$ have zero eigenvalues. For simplicity let us assume $\ell = 1$. The domain of integration $\boldsymbol{X}$ spanned by the complete set of eigenvectors can be decomposed into a one-dimensional space $\boldsymbol{X}^1$ spanned by $\boldsymbol{\Psi}_0$ and an infinite dimensional space $\boldsymbol{X}^\infty$ of codimension 1. Under the change (5.22) the expansion of the action functional reads

$$S(x) = S(q) + c_0 u^0 + \frac{1}{2}\sum_{k=1}^{\infty} \alpha_k (u^k)^2 + \mathcal{O}(|u|^3) \tag{5.23}$$

with

$$c_0 = \int_{\boldsymbol{T}} dt \frac{\delta S}{\delta q^j(t)} \Psi_0^j(t). \tag{5.24}$$

Remark: In finite dimension, according to the Morse lemma, there is a nonlinear change of variable which can be used to remove the terms of order greater than 2 in a Taylor expansion. In infinite dimension ther is no general prescription for removing $\mathcal{O}(|u|^3)$.

The integral over u^0 contributes a δ-function to the propagator $\delta(c_0/h)$. The propagator vanishes unless the conservation law

$$\frac{1}{h}\int_{\boldsymbol{T}} dt \frac{\delta S}{\delta q^j(t)} \boldsymbol{\Psi}_0^j(t) = 0 \tag{5.25}$$

is satisfied.

In conclusion conservation laws appear in the classical limit of quantum physics. It is not an anomaly for a quantum system to have less symmetry than its classical limit.

5.3 Caustics

In section 5.2 we approached the crossroad $U^{2D}_{\mu,\nu}$ from $T_q\mathcal{T}_{\mu,\nu}\mathbb{M}^D$. Now we approach the crossroad from T_qU^{2D}. As we approach quantum physics from classical physics, we see that a caustics (the envelope of a family of classical paths) is "softened up" by quantum physics.

Physics abound in caustics. We quote only four examples corresponding to the boundary conditions (initial or final, position or momentum) we have been discussing in the Appendix IE.

(i) The soap bubble problem [3]. 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. 5.2. 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 tan 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.

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, for instance, the scattering of particles by a repulsive Coulomb potential. For other examples see [4].

Let q and q^{Δ} be two solutions of the same Euler-Lagrange equation with slightly different boundary conditions at t_b, i.e. $q \in T_q\mathcal{P}_{\mu,\nu}\mathbb{M}$ and $q^{\Delta} \in T_{q^{\Delta}}\mathcal{P}_{\mu^{\Delta},\nu}\mathbb{M}$.

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

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 $(p_a,\, b^{\Delta})$ 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

Fig. 5.3. A flow on configuration space of charged particles in a repulsive Coulomb potential.

phase equal to $-\pi/2$; both limits are infinite and their sum is not defined.

We compute $K(b^{\triangle}, t_b; p_a, t_a)$ by expanding S around q, using (5.6) – and possibly higher derivatives if the third variation is singular. The calculation requires some care [see reference [5] for details] because $q(t_b) \neq b^{\triangle}$; in other words q is not a critical point of the action restricted to the space of paths such that $x(t_b) = b^{\triangle}$. We approach the intersection in a direction other than a tangent to $\mathcal{U}$.

Fig. 5.4. (p_a, b) are conjugate along q; $(p_a, b_{\triangle})$ are not conjugate along $q_{\triangle}$.

As before we make the change (5.9) (5.10) of variable $\xi \mapsto u$ which diagonalizes $S''(q) \cdot \xi\xi$. Again we decompose the domain of integration in the u-variable

$$\boldsymbol{X} = \mathbb{X}^1 \times \mathbb{X}^\infty.$$

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

$$I(\nu, c) = \int_{I\!R} du^0 \exp\left(\imath\left(cu^0 - \frac{\nu}{3}(u^0)^3\right)\right) = \nu^{-1/3}\mathrm{Ai}(\nu^{-1/3}c) \tag{5.26}$$

where

$$\nu = \frac{\pi}{h}\int_{\mathbf{T}} \mathrm{d}r \int_{\mathbf{T}} \mathrm{d}s \int_{\mathbf{T}} \mathrm{d}t \frac{\delta^3 S}{\delta q^\alpha(r)\delta q^\beta(s)\delta q^\gamma(t)} \psi_0^\alpha(r)\psi_0^\beta(s)\psi_0^\gamma(t) \tag{5.27}$$

$$c = -\frac{2\pi}{h}\int_{\mathbf{T}} \mathrm{d}t \frac{\delta S}{\delta q(t)} \cdot \psi_0(t)(b^\Delta - b) \tag{5.28}$$

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 $v^2 = \nu^{-1/3}c$

$$\mathrm{Ai}(\nu^{-1/3}c) \simeq \begin{cases} 2\sqrt{\pi}v^{-1/4}\cos\left(\frac{2}{3}v^2 - \frac{\pi}{4}\right) & \text{for } v > 0 \\ \sqrt{\pi}(-v)^{-1/4}\exp\left(-\frac{2}{3}v^3\right) & \text{for } v < 0 \end{cases} . \tag{5.29}$$

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 [5] and [4].

5.4 glory scattering

Backward scattering of light, very close to the direction of the incoming rays has a long and interesting history (see for instance [6] 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 [7], [5].

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

$$d\sigma_{c\ell}(\Omega) = 2\pi \, B(\theta) \, dB(\theta) \tag{5.30}$$

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

$$d\sigma_{c\ell}(\Omega) = B(\Theta) \left. \frac{dB(\Theta)}{d\Theta} \right|_{\Theta=\theta} \frac{d\Omega}{\sin\theta} \tag{5.31}$$

abbreviated henceforth

$$d\sigma_{c\ell}(\Omega) = B(\theta) \frac{dB(\theta)}{d\theta} \frac{d\Omega}{\sin\theta} \, . \tag{5.32}$$

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

$$\theta = \Theta(B_g) \text{ is } 0 \text{ or } \pi \, , \tag{5.33}$$

implying $\sin\theta = 0$, and making (5.32) useless.

The classical glory scattering cross-section is infinite 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 $-B_g + \delta B$ exit with approximately the same angles, namely $\pi +$ terms of order $(\delta B)^3$.

The glory cross-section can be computed [7], [5] using the methods presented in sections II and III. The result is

$$d\sigma(\Omega) = 4\pi^2 \, h^{-1} \, |p_a| \, B^2(\theta) \, \frac{dB(\theta)}{d\theta} \, J_0(2\pi \, h^{-1} \, |p_a| \, B(\theta) \, \sin\theta)^2 \, d\Omega \tag{5.34}$$

where J_0 is the Bessel function of order 0.

A similar calculation [8], [5], [6] gives the WKB cross-section for polarized glories of massless waves in curved spacetimes

$$d\sigma(\Omega) = 4\pi^2 \, \lambda^{-1} \, B_g^2 \, \frac{dB}{d\theta} \, J_{2s}(2\pi \, \lambda^{-1} \, B_g \, \sin\theta)^2 \, d\Omega \tag{5.35}$$

$s = 0$ for scalar waves; at glory $J_0(0)^2 \neq 0$
$s = 1$ for electromagnetic waves; at glory $J_2(0)^2 = 0$
$s = 2$ for gravitational waves; at glory $J_4(0)^2 = 0$.
λ is the wave length of the incoming wave.

Equation (5.35) matches perfectly with the numerical calculations [8] of R. Matzner based on the partial wave decomposition method.

Fig. 5.5.

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

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

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

analytic cross section: dashed line
numerical cross section: solid line

5.5 Tunneling

A quantum transition between two points **a** and **b** not connected by a classical path is called tunneling[9]: quantum particles can go through potential barriers, *e.g.* in nuclear α-decay, α-particles leave a nucleus although they are inhibited by a potential barrier. To prepare the study of semiclassical tunneling we recall the finite dimensional case, namely the stationary phase approximation† when the critical point of the phase

† see for instance [10] Vol. I, p.593 and [11].

lies outside the domain of the integration.

Introduction

In its simplest form, the stationary phase approximation is an asymptotic approximation for large λ of integrals of the following form

$$F(\lambda) = \int_{\mathbb{X}} d\mu(x)\ h(x)\ \exp\left(\imath\lambda f(x)\right), \tag{5.36}$$

where h is a real-valued smooth function of *compact* support on the D-dimensional Riemannian manifold $\boldsymbol{X}$ with volume elements $d\mu(x)$ and where the critical points of f (i.e., the solutions of $f'(y) = 0,\ y \in \boldsymbol{X}$) are assumed to be nondegenerate, that is the determinant of the Hessian $\frac{\partial^2 f}{\partial x^i \partial^j}$ does not vanish at the critical point $x = y$. In this simple case

$$F(\lambda) \approx \mathcal{O}(\lambda^{-N}), \qquad \text{for any } N \text{ if } f \text{ has no critical point on the support of } h \tag{5.37}$$

$$F(\lambda) \approx \mathcal{O}(\lambda^{-D/2}), \qquad \text{if } f \text{ has a finite number of nondegenerate critical points on the support of } h. \tag{5.38}$$

These results have been generalized when the critical point $y \in$ supp h is degenerate†. We recall the following case paving the way for semiclassical tunneling.

Stationary phase approximation when the integrand does not vanish on the boundary $\partial\boldsymbol{X}$ of the domain of integration $\boldsymbol{X}$.

The simple results (5.37) and (5.38) are obtained by integrating (5.35) by parts, under the assumption that the boundary terms vanish. Now the boundary term do not vanish. For example‡ let $\boldsymbol{X} = [a, b] \subset I\!R$, then

$$F(\lambda) = \frac{1}{\imath\lambda}\ \frac{h(x)}{f'(x)}\ \exp\left(\imath\lambda f(x)\right)\Big|_a^b - \frac{1}{\imath\lambda}\int_a^b \left(\frac{h(x)}{f'(x)}\right)'\ \exp\left(\imath\lambda f(x)\right)\ dx. \tag{5.39}$$

After N integration by parts, the boundary terms consist of the polynomial in $(\imath\lambda)^{-1}$ of order N; as in the simple case the remaining integral

† See section (**??**) and (**??**) for the infinite dimensional counterpart of this case.
‡ For the integration by parts of the general case, see [11]. The example is sufficient for computing the powers of λ.

is of order λ^{-N} for any N if f has no critical point in the domain of integration, and is of order $\lambda^{-D/2}$ otherwise. Therefore the leading term for large λ is the boundary term in (5.39).

The leading term of $F(\lambda)$ in equation (5.38) is, after integration by parts, the boundary term. It can be rewritten† as an integral over the $(D-1)$ dimensional boundary $\partial\boldsymbol{X}$, namely

$$F(\lambda) \approx \frac{1}{\imath\lambda} \int_{\partial\mathbb{X}} h(x)\ \exp\left(\imath\lambda f(x)\right)\ \boldsymbol{\omega} \cdot\ d\boldsymbol{\sigma}(x), \tag{5.40}$$

where the boundary $\partial\boldsymbol{X}$ is regular and compact, $\boldsymbol{\omega}$ is the derivation at x defined by

$$\boldsymbol{\omega}(x) := \frac{\mathbf{v}(x)}{|\mathbf{v}(x)|^2}, \quad \text{with} \quad \mathbf{v}(x) = g^{ij}(x)\ \frac{\partial f}{\partial x^i}\ \frac{\partial}{\partial x^j}, \tag{5.41}$$

and $d\boldsymbol{\sigma}$ is the $(D-1)$ dimensional surface element on $\partial\boldsymbol{X}$. The asymptotic expression (5.40) can in turn be obtained by the stationary phase method. The integral is either of order $\lambda^{-1}\ \lambda^{-N}$ for any N if $f|_{\partial\mathbb{X}}$ has no critical point, and of order $\lambda^{-1}\ \lambda^{-(D-1)/2}$ otherwise.

The phase f restricted to $\partial\boldsymbol{X}$ obtains its extrema when the components of grad$f$ in T_yX (with $y \in \partial\boldsymbol{X}$) vanish, i.e. when grad$f(y)$ is normal to $\partial\boldsymbol{X}$.

The wedge problem has a long and distinguished history‡. In 1896, Sommerfeld, then a *Privat-Dozent*, computed the diffraction of light from a perfectly reflecting knife edge – i.e. a wedge with external angle $\theta = 2\pi$. He used an Ansatz suggested by Riemann's computation of the potential of a point charge outside a conducting wedge of external angle $\theta = \mu\pi/\nu$ with μ/ν rational.

In 1938, at the occasion of Sommerfeld seventieth birthday, Pauli dedicated to his "old teacher" a paper on wedges.

The wedge is a boundary value problem whose solution exploit the method of images, Riemann surfaces for multivalued functions, properties of special functions etc. . . . . In brief, a combination of powerful an-

† Rewriting the boundary terms as an integral over the boundary is a classic exercise in integration over Riemannian spaces; see details for instance in [11] pp. 228-329
‡ Some historical references can be found in [1] (see bibliography) dedicated to John Archibald Weeler at the occasion of his seventienth birthday.

Fig. 5.6. The source is at **a** with coordinates (R', ϕ'), the detector is at **b** with coordinates at (R, ϕ). The wedge angle θ is the external angle. When $\theta = 2\pi$ the wedge is a half plane barrier called a knife edge.

alytic tools. It is therefore amazing that L.S. Schulman[12] found a simple exact path integral representing the probability amplitude $K(\mathbf{b}, t; \mathbf{a})$ that a particle at **a** at time $t = 0$ be found at **b** at time t, when a knife edge precludes the existence a classical path from **a** to **b**.

The mathematical similarity† of the three techniques used by Riemann, Sommerfeld, and Schulman is often mentioned when interferences occurring in the two-slit experiment is invoked for introducing path integration – but this similarity is rarely used in the context of diffraction.

Schulman's result is challenging, but upon reflection not unexpected; functional integration is ideally suited for solving boundary value problems. Indeed it incorporates the boundary conditions in the choice of its domain of integration, whereas boundary conditions in differential calculus are *additional* requirement satisfied by a solution of a PDE whose compatibility has to be checked. Moreover a PDE states only local relationships between a function and its derivative, whereas the domain of

† The similarity is spelled out in [11].

integration of a path integrals consist of paths which probe the global properties of their ranges.

Schulman's Computation of the Knife Edge Tunneling

Consider a free particle of mass unity, which cannot pass through a thin barrier along the positive axis.

Fig. 5.7. The point **c** is visible from **a** and **b**. A path **ac** is called "direct", a path **adc**, which reaches **c** after a reflection at **d** is called "reflected".

The knife edge problem can be solved in $\mathbb{R}^2$ without loosing its essential characteristics. The probability amplitude $K(\mathbf{b}, t; \mathbf{a})$ that a particle at **a** at time $t = 0$ be found at **b** at time t can always be expressed as the following integral on $\mathbb{R}^2$

$$K(\mathbf{b}, t; \mathbf{a}) = \int_{\mathbb{R}^2} d^2c\ K(\mathbf{b}, t - t_c; \mathbf{c})\ K(\mathbf{c}, t_c; \mathbf{a}), \tag{5.42}$$

for an arbitrary intermediate t_c. It is convenient to choose t_c equal to the time a free particle going from **a** to **0**, to **b**, reaches **0**, the edge of the knife. When **c** is visible both from **a** and **b**, (located as in the figure) there are direct contributions

$$K_D(\mathbf{b}, t - t_c; \mathbf{c}) = (2\pi\imath\hbar(t - t_c))^{-1}\ \exp\left(\imath\frac{|\mathbf{b} - \mathbf{c}|^2}{2\hbar(t - t_c)}\right), \tag{5.43}$$

$$K_D(\mathbf{c}, t_c; \mathbf{a}) = (2\pi\imath\hbar t_c)^{-1}\ \exp\left(\imath\frac{|\mathbf{c} - \mathbf{a}|^2}{2\hbar t_c}\right), \tag{5.44}$$

and a reflected contribution

$$K_R(\mathbf{c}, t_c; \mathbf{a}) = (2\pi\imath\hbar t_c)^{-1}\ \exp\left(\imath\frac{|\mathbf{c}' - \mathbf{a}|^2}{2\hbar t_c}\right), \tag{5.45}$$

where $\mathbf{c}'$ is symmetric to **c** with respect to the barrier plane. Let $K_{DD}(\mathbf{b}, t; \mathbf{a})$ be the probability amplitude obtained by inserting (5.43) and (5.44) into (5.42), and $K_{DR}(\mathbf{b},t;\mathbf{a})$ be the probability amplitude obtained by inserting (5.43) and (5.45) into (5.42). It is understood that each term appears only in its classically allowed region. The total probability amplitude $K(\mathbf{b},t;\mathbf{a})$ is a linear combination of K_{DD} and K_{DR}. Schulman considers two possible linear combination

$$K^{\mp}(\mathbf{b},t;\mathbf{a}) = K_{DD}(\mathbf{b},t;\mathbf{a}) \mp K_{RD}(\mathbf{b},t;\mathbf{a}). \tag{5.46}$$

After some calculations, he obtains

$$K^{\mp}(\mathbf{b},t;\mathbf{a}) = K_0 \left(e^{-\imath m^2}\ h(-m) \mp e^{-\imath n^2}\ h(-n) \right), \tag{5.47}$$

where

$$K_0 = \frac{1}{2\pi \imath \hbar t}\ \exp\left(\frac{\imath}{2\hbar t} (|\mathbf{a}\ \mathbf{0}|^2 + (\mathbf{0}\ \mathbf{b})^2) \right) \tag{5.48}$$

with

$$m = (2/\hbar\gamma)^{1/2} v \sin\omega_2\ , \qquad n = (2/\hbar\gamma) v^2 \sin\omega_1 \tag{5.49}$$

$$\omega_2 = \frac{1}{2}(\phi' - \phi) - \frac{\pi}{2}\ , \qquad \omega_1 = \frac{1}{2}(\phi' + \phi) \tag{5.50}$$

$$\gamma = t_c^{-1} + (t - t_c)^{-1}\ , \qquad v = |\mathbf{a}\ \mathbf{0}|/t_c = |\mathbf{0}\ \mathbf{b}|/(t - t_c) \tag{5.51}$$

and

$$h(m) = (\pi)^{-1/2} \exp(-\imath\pi/4) \int_{-\infty}^{m} \exp(\imath t^2)\ dt.$$

The propagators $K^{\mp}$ are identical to the propagators obtains by Carslaw who 1899 had been used by Sommerfeld to continue his investigation of the knife edge problem. The propagator K^{-} consists of two contributions which interfere destructively on the far side of the knife; it can be said to vanish on the knife, or to satisfy Dirichlet boundary condition. The propagator K^{+} consists of the sum of two contributions whose normal derivatives (perpendicular to the knife) interfere destructively on far side of the knife; it can be said to satisfy Neumann boundary conditions.

Note that for $\phi' - \phi < \pi$, there is a straight line in the space of allowed paths and the stationary phase approximation of $K(\mathbf{b},t;\mathbf{a})$ is the free propagator K_0 in $I\!R^2$ proportional to $\hbar^{-1}$. If not the stationary phase approximation is dominated by the boundary terms and $K(\mathbf{b},t;\mathbf{a})$ is of order $\hbar^{1/2}$.

Independently of Schulman, F.W. Wiegel and J. Boersma[13] and Amar Shiekh have solved the knife edge problem by other novel path integral techniques. Wiegel and Boersma base their derivation on results obtained in the solution of the polymer problem, another case in which the boundary of the domain of integration of a path integral determines the solution.

Shiekh bases his derivation on the properties of free propagators on a 2-sheeted Riemann surface, constructed as a linear combination of Aharonov-Bohm propagators for different fluxes.

Chapter 5 is based on two articles "Physics on and near Caustics" by the authors of this book which have appeared in the following proceedings:

- *Functional Integration: Basics and Applications.* Eds. C. DeWitt-Morette, P. Cartier, and A. Folacci; a NATO-ASI Series B (Physics), Vol. 361 (Plenum Press, New York, 1997).
- RCTP Proceedings of the second Jagna Workshop (January 1998).

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