The Hamilton–Jacobi Equation, Semiclassical Asymptotics, and Stationary Phase

Main source: A. Uribe, Cuernavaca Lectures, Appendices B and C and parts of Section 2
(first item on our Background Reading page)

**Stationary Phase**

Consider \[ I(t) \equiv \int_{\mathbb{R}^n} e^{it\phi(x)}a(x) \, dx, \]
\(\phi\) smooth and real-valued \((\phi \in C^\infty_\mathbb{R}(\mathbb{R}^n))\), \(a\) smooth and compactly supported \((a \in C^\infty_0(\mathbb{R}^n))\), \(t \to +\infty\).
(No vector boldface this time; \(n\) may not be \(d\).

*Intuition:* \(I\) is very small for large \(t\), because the integrand oscillates rapidly — except in regions where \(\phi\) is nearly constant!

*Definition:* Points of stationary phase are critical points of \(\phi\) \((\nabla \phi(x_0) = 0)\).
\[ I(t) \equiv \int_{\mathbb{R}^n} e^{it\phi(x)} a(x) \, dx, \quad \nabla \phi(x_0) = 0. \]

**Nonstationary Phase Theorem.** If \( \phi \) has no critical points in a neighborhood of \( \text{supp} \, a \) (i.e., \( a = 0 \) at and near any \( x_0 \)), then \( I(t) = O(t^{-N}) \) for any \( N \).

**Proof:** Integrate by parts forever! (\( \chi = \text{cutoff.} \))

\[ ae^{it\phi} = \frac{a}{it} L(e^{it\phi}) \quad \text{where} \quad L \equiv \frac{\chi}{|\nabla \phi|^2} \nabla \phi \cdot \nabla; \]

\[ I(t) = \int ae^{it\phi} \, dx = \frac{i}{t} \int e^{it\phi} L^t a \, dx, \]

an integral of same form. Repeat to get \( \frac{1}{t^N} \).

**Corollary** \( (\phi(x) = k \cdot x) \): The Fourier transform of a smooth function is a function of rapid decrease.

**Remark:** Compact support is too strong; all we need is that all endpoint terms vanish. But smoothness of \( a \) and \( \phi \) is fundamental.
\[ I(t) = \int_{\mathbb{R}^n} e^{it\phi(x)} a(x) \, dx, \quad \nabla \phi(x_0) = 0. \]

**Stationary Phase Theorem (quadratic case).**

Consider \( \phi(x) = \frac{1}{2} x \cdot Ax, \det A \neq 0 \); \( x_0 = 0 \). Then

\[ I(t) \sim \left( \frac{2\pi}{t} \right)^{n/2} \frac{e^{i\pi \sigma/4}}{\sqrt{|\det A|}} \sum_{j=0}^{\infty} b_j(a)(0)t^{-j}, \]

where \( b_j \) is a differential operator of order \( 2j \) \( (b_0 = 1) \) and \( \sigma \) is the signature of \( A \) (number of positive eigenvalues minus number of negative eigenvalues).

**Proof:** Go to a frame where \( A \) is diagonal and treat each dimension separately: For \( A \in \mathbb{R}, A > 0, \mu > 0, \)

\[ \int e^{-\mu Ax^2/2} a(x) \, dx = \frac{1}{\sqrt{2\pi\mu A}} \int e^{-k^2/2\mu A} \hat{a}(k) \, dk \]

(by Parseval’s equation and the Gaussian Fourier transform formula). Since \( \hat{a} \) has rapid decrease, we can analytically continue to \( \mu = -it, t > 0: \)

\[ \int e^{itAx^2/2} a(x) \, dx = \frac{e^{i\pi/4}}{\sqrt{2\pi t|A|}} \int e^{-ik^2/2tA} \hat{a}(k) \, dk. \]
For $A < 0$ you get $e^{-i\pi/4}$ instead. So in dimension $n$

$$I(t) = \int e^{itx \cdot Ax/2} a(x) \, dx$$

$$= \frac{e^{i\pi\sigma/4}}{(2\pi t)^{n/2} \sqrt{|\det A|}} \int e^{-ik \cdot A^{-1}k/2t} \hat{a}(k) \, dk.$$ 

Expand

$$e^{-ik \cdot A^{-1}k/2t} \sim 1 - t^{-1} k \cdot A^{-1}k/2 + \cdots + t^{-j} O(k^{2j}) + \cdots$$

and interpret $j$th term as Fourier representation of some $2j$th derivatives of $a(x)$ evaluated at 0.

**Remark:** The series (usually) does not converge, but it is asymptotic: the remainder after $N$ terms is $O(t^{-N-1})$.

**Remark:** For an integral over a finite interval there will be additional terms coming from the endpoints. More generally, if $a(x)$ is only piecewise smooth there will be extra terms associated with each singularity.
Definitions: Critical point $x_0$ is nondegenerate if

$$\text{Hess}_{x_0} \phi \equiv \det \left( \frac{\partial^2 \phi}{\partial x_i \partial x_j} (x_0) \right) \neq 0.$$  

(Also use $\text{Hess}_{x_0} \phi$ for the matrix itself.)

Morse’s Lemma. In the vicinity of a nondegenerate critical point one can choose coordinates so that

$$\phi(x(y)) = \phi(x_0) + \frac{1}{2} \sum_{j=1}^{n} \Lambda_j y_j^2$$

($\Lambda_j$ being the eigenvalues of $\text{Hess}_{x_0} \phi$).

Note: No “$+ O(y^3)$”. Cf.

mean value theorem \hspace{1cm} $f(x) = f(0) + f'(c)x$

vs. Taylor’s theorem \hspace{1cm} $f(x) = f(0) + f'(0)x + O(x^2)$.

Sketch of Proof: Use multidimensional Taylor’s theorem with remainder (in integral form) to write

$$\phi(x) = \phi(x_0) + \frac{1}{2} (x - x_0) \cdot H(x)(x - x_0)$$

for some $H(x)$. Then use implicit function theorem on the mapping of matrices $M \mapsto M^t(\text{Hess}_{x_0} \phi) M$ to write

$$H(x) = \left( M(H(x)) \right)^t \left( \text{Hess}_{x_0} \phi \right) M(H(x))$$

and hence

$$y \equiv M(H(x))(x - x_0).$$
\[ I(t) \equiv \int_{\mathbb{R}^n} e^{it\phi(x)}a(x) \, dx, \quad \nabla \phi(x_0) = 0. \]

Put together the three theorems to get:

**Stationary Phase Theorem.** Assume \( \phi \in C^\infty_c(\mathbb{R}^n) \), \( a \in C^\infty_c(\mathbb{R}^n) \), and the only critical points of \( \phi \) in some neighborhood of \( \text{supp } a \) are nondegenerate (and hence isolated); call them \( x_{01}, \ldots, x_{0K} \). Then as \( t \to \infty \)

\[
I(t) \sim \left( \frac{2\pi}{t} \right)^{n/2} \sum_{k=1}^{K} \frac{e^{i\pi \sigma_k/4} e^{it\phi(x_{0k})}}{\sqrt{\text{Hess}_{x_{0k}}} \phi} \times \left[ a(x_{0k}) + \sum_{j=1}^{\infty} b^k_j(a)(x_{0k})t^{-j} \right],
\]

where \( b^k_j \) are certain PDOs and \( \sigma_k \) is the signature of \( \text{Hess}_{x_{0k}} \phi \).

See (for instance) S. Zelditch, [math.SP/0111078](math.SP/0111078), for a Feynman-diagram algorithm for \( b^k_j \).

**Remark:** Often in practice the critical points are not isolated. Instead, there may be a whole submanifold \( \mathcal{T} \) of critical points, with \( \text{Hess} \phi \) degenerate in directions tangent to \( \mathcal{M} \). But if it’s nondegenerate in the normal directions one can apply stationary phase in those directions and integrate the result over \( \mathcal{T} \).
**Hamiltonian classical mechanics**

Let $H(x, p)$ be a (smooth) real-valued function defined on [a subset of, or manifold like] $\mathbb{R}^{2d}$ (phase space). Usually, $H$ is a second-degree polynomial in $p$. Main example:

$$H(x, p) = \frac{p^2}{2m} + V(x).$$

Then

$$\frac{dx}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial x}$$

is a first-order ODE system with solutions (Hamiltonian flow)

$$(x(t), p(t)) = \Phi_t(x_0, p_0)$$

for initial data $(x(t), p(t)) = (x_0, p_0)$.

All this is equivalent to a Newtonian equation of motion (second-order ODE for $x$) plus a definition of $p$ in terms of $\dot{x}$ (or vice versa).

Energy is conserved:

$$\frac{d}{dt}H(x(t), p(t)) = \frac{\partial H}{\partial x} \frac{dx}{dt} + \frac{\partial H}{\partial p} \frac{dp}{dt} = 0.$$  

So $H(x(t), p(t)) \equiv E$. 

7
Two PDEs associated with $H$

Schrödinger equation (2nd order, linear):
Replace $p$ by $-i\hbar\nabla$, $E$ by $+i\hbar \frac{\partial}{\partial t}$.

$$i\hbar \frac{\partial u}{\partial t} = H u = -\frac{\hbar^2}{2m} \nabla^2 u + Vu.$$  

Time-independent version: $-\frac{\hbar^2}{2m} \nabla^2 u + Vu = Eu$.

Hamilton–Jacobi equation (1st order, nonlinear):
Replace $p$ by $\nabla S$, $E$ by $-\frac{\partial S}{\partial t}$, where $S(t, x)$ is the unknown.

$$-\frac{\partial S}{\partial t} = H(x, \nabla S) = \frac{|\nabla S|^2}{2m} + V(x).$$  

Time-independent version: $H(x, \nabla S) = E$.

Semiclassical ansatz: $u(t, x) = A(t, x; \hbar) e^{iS(t, x)/\hbar}$, $\hbar \to 0$, later $A \sim A_0 + \hbar A_1 + \hbar^2 A_2 + \cdots$. You get

$$0 = A \left[ \frac{\partial S}{\partial t} + \frac{1}{2m} |\nabla S|^2 + V \right]$$

$$- i\hbar \left[ \frac{\partial A}{\partial t} + \frac{1}{m} \nabla A \cdot \nabla S + \frac{1}{2m} A \nabla^2 S \right] - \frac{\hbar^2}{2m} \nabla^2 A.$$  

So solving HJ is first step in an $\hbar$ expansion.
Relation between HJ and classical mechanics

(1) Assume we have a (local) solution of HJ,
\[- \frac{\partial S(t, x)}{\partial t} = H(x, \nabla S(t, x)),\]
and a (local) curve \(x(t)\) satisfying
\[\frac{dx}{dt} = \frac{\partial H}{\partial p}(x(t), \nabla S(t, x(t))) \equiv \frac{1}{m} \nabla S(t, x(t)).\]

Then \((x(t), \nabla S(t, x(t)))\) is a trajectory of the Hamiltonian flow (with \(p(t) = \nabla S(t, x(t))\)).

**Proof:** \(\frac{dx}{dt} = \frac{\partial H}{\partial p}\) is satisfied by assumption. Why \(\frac{dp}{dt} = -\frac{\partial H}{\partial x}\)? Calculate
\[\frac{dp_i}{dt} = \frac{\partial^2 S}{\partial t \partial x_i} + \sum_j \frac{\partial^2 S}{\partial x_j \partial x_i} \frac{dx_j}{dt}.\]

And differentiate HJ:
\[\frac{\partial^2 S}{\partial x_i \partial t} = - \frac{\partial H}{\partial x_i} - \sum_j \frac{\partial H}{\partial p_j} \frac{\partial^2 S}{\partial x_i \partial x_j}.\]

Compare: \(\frac{dp_i}{dt} = - \frac{\partial H}{\partial x_i}\).

**Corollary:** Entrance of the Lagrangian.
\[\frac{d}{dt} S(t, x(t)) = \frac{\partial S}{\partial t} + \dot{x} \cdot \nabla S = -H + \dot{x} \cdot p \equiv L(x(t), \dot{x}(t)).\]
(2) Conversely, assume we know the flow $\Phi_t$. The previous corollary suggests that we should get solutions of HJ by integrating $L$ along the trajectories. Indeed, for given $(t, x, x_0)$ in a sufficiently small neighborhood in $\mathbb{R}^{1+2d}$, the two-point boundary problem

$$x(0) = x_0, \quad x(t) = x$$

for the (Newtonian) equation of motion will have a unique solution $x(t)$. Define

$$S(t, x; x_0) = \int_0^t L(x(u), \dot{x}(u)) \, du.$$  

Then $S$ solves HJ. (Note that arbitrary initial data $S_0(x_0)$ could be added.)

**Proof:** is somewhat complicated. See


**Corollary:** Initial and final momenta.

$$p(t) = \nabla_x S(t, x; x_0).$$

By symmetry,

$$p(0) = -\nabla_{x_0} S(t, x; x_0) + \nabla S_0(x_0), \text{ in general}.$$
(3) Return to (1) and assume we have a parametrized family of (local) solutions of HJ, $S(t, x; p_0)$, such that $S(0, x; p_0) = x \cdot p_0$. Then any flow trajectory, $(x(t), p(t))$, running through the domain of $S$ is of the form described in (1), with $p(0) = p_0$.

**Proof:** Define $\tilde{x}(t)$ by

$$\frac{d\tilde{x}(t)}{dt} = \frac{\partial H}{\partial p}(\tilde{x}(t), \nabla S(t, \tilde{x}(t); p(0)),$$

and define $\tilde{p}(t) = \nabla S(t, \tilde{x}(t); p(0))$. By (1), $(\tilde{x}, \tilde{p})$ is a trajectory. Its initial data are $(x(0), p(0))$, because $\tilde{p}(0) = \nabla S(0, \tilde{x}(0); p(0)) = \nabla_{x(0)}[x(0) \cdot p(0)] = p(0)$. Therefore, $(\tilde{x}, \tilde{p}) = (x, p)$ for all $t$, since trajectory is unique.

**Remark:** In the context of (2), these solutions are those with $S_0(x_0) = x_0 \cdot p_0$. It follows that

$$p(0) = -\nabla_{x_0} S(t, x; p_0) + \nabla S_0(x_0)$$

$$= -\nabla_{x_0} S(t, x; p_0) + p_0,$$

but we know $p(0) = p_0$, so $\nabla_{x_0} S(t, x; p_0) = 0$, as the notation implies.
(4) Let’s be more precise about the two-point boundary problem. We have a flow

\[ \Phi_t(x_0, p_0) = (x, p) \equiv (x(t, x_0, p_0), p(t, x_0, p_0)). \]

Assume that for each \((t, p_0)\) in some open set the map \(x_0 \mapsto x(t, x_0, p_0)\) is a diffeomorphism, so it has inverse \(x \mapsto x_0(t, x, p_0)\). In words, \(x_0\) is the initial position of a particle of initial momentum \(p_0\) that at time \(t\) arrives at \(x\). (In (2) the roles of \(x_0\) and \(p_0\) were interchanged.) We now claim

\[ x_0(t, x, p_0) = \nabla_{p_0} S(t, x; p_0). \]

**PROOF:** Write the claim as

\[ x_0(t, x, p_0) = \nabla_{p_0} S(t, x(t, x_0, p_0); p_0). \]

It holds at \(t = 0\):

\[ \nabla_{p_0} S(0, x(0); p_0) = \nabla_{p_0} [x_0 \cdot p_0] = x_0. \]

Therefore, it holds for all \(t\), because the derivative of the expression vanishes, by calculation like that in (1):

\[ \frac{d}{dt} x_{0i} = \frac{\partial^2 S}{\partial t \partial p_i} + \sum_j \frac{\partial^2 S}{\partial x_j \partial p_i} \frac{dx_j}{dt}, \]

but differentiating HJ yields

\[ \frac{\partial^2 S}{\partial p_i \partial t} = - \sum_j \frac{\partial H}{\partial p_j} \frac{\partial^2 S}{\partial p_i \partial x_j}, \]

and it all cancels.
Recapitulation

\[ S(t, x; x_0) = \int_0^t L \text{ satisfies} \]

\[ p = \nabla_x S(t, x; x_0), \quad p_0 = -\nabla_{x_0} S(t, x; x_0). \]

In the language of Goldstein, *Classical Mechanics*, $-S(t, x, ; x_0)$ is a generating function of type $F_1$ for $\Phi_t$ regarded as a canonical transformation from the old variables $(x_0, p_0)$ to the new variables $(x, p)$.

\[ S(t, x; p_0) = \int_0^t L + x_0 \cdot p_0 \text{ (which is actually independent of } x_0 \text{ and has initial data } S(0, x; p_0) = x \cdot p_0) \text{ satisfies} \]

\[ p = \nabla_x S(t, x; p_0), \quad x_0 = \nabla_{p_0} S(t, x; p_0). \]

So $-S(t, x; p_0)$ is a generating function of type $F_3$ for $\Phi_t$.

**Remark:** Therefore, contrary to appearance, $S(t, x; x_0)$ does not approach 0 as $t \to 0$ if $x \neq x_0$. The reason is that if the particle gets from $x_0$ to $x$ in a very short time, then $L$ is very large!

\[ S(0, x; x_0) = (x - x_0) \cdot p_0. \]
THE TRANSPORT EQUATION

Recall that to solve the Schrödinger equation (for $H = \frac{P^2}{2m} + V$) through order $\hbar^1$ we need to solve

$$\frac{\partial A}{\partial t} + \frac{1}{m} \nabla A \cdot \nabla S + \frac{1}{2m} A \nabla^2 S = 0.$$  

But because $S$ solves HJ, we have

$$\nabla S = p = m \dot{x}.$$  

Therefore,

$$\left( \frac{\partial}{\partial t} + \frac{1}{m} \nabla S \cdot \nabla \right) A = \left( \frac{\partial}{\partial t} + \dot{x} \cdot \nabla \right) A = \frac{dA}{dt}(x(t)),$$

and we can solve for $\ln A$ (actually, $\ln A_0$) by integrating along the classical trajectories!

$$A_0(x) = \exp \left[ -\frac{1}{2m} \int_0^t \nabla^2 S(u, x(u)) \, du \right]$$

(where $x(0) = x_0$, $x(t) = x$). Higher-order terms $\hbar^n A_n$ can be calculated in the same way.

Alternative solution: Van Vleck determinant.

$$A_0(x) = \sqrt{|\det \nabla_x \nabla_{x_0} S|}.$$  

This determinant becomes infinite at places $x$ where the flow ceases to be a diffeomorphism (trajectories emerging from $x_0$ intersect for the first time).