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 $\quad I(t) \equiv \int_{\mathbf{R}^n} e^{it\phi(x)} a(x)\,dx,$

ϕ smooth and real-valued ($\phi \in C^\infty_{\mathbf{R}}(\mathbf{R}^n)$), a smooth and compactly supported ($a \in C^\infty_0(\mathbf{R}^n)$), $t \to +\infty$. (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 ϕ is nearly constant!

Definition: *Points of stationary phase* are *critical points* of ϕ $\quad (\nabla\phi(x_0) = 0)$.

$$I(t) \equiv \int_{\mathbf{R}^n} e^{it\phi(x)} a(x)\,dx, \qquad \nabla\phi(x_0) = 0.$$

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

Proof: Integrate by parts forever! ($\chi =$ cutoff.)

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

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

an integral of same form. Repeat to get $\dfrac{1}{t^N}$.

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 ϕ is fundamental.

$$I(t) \equiv \int_{\mathbf{R}^n} e^{it\phi(x)} a(x)\, dx, \qquad \nabla\phi(x_0) = 0.$$

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* σ *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 $A \in \mathbf{R}$, $A > 0$, $\mu > 0$,

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

(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

$$\begin{aligned} I(t) &= \int e^{itx\cdot Ax/2} a(x)\,dx \\ &= \frac{e^{i\pi\sigma/4}}{(2\pi t)^{n/2}\sqrt{|\det A|}} \int e^{-ik\cdot A^{-1}k/2t} \hat{a}(k)\,dk. \end{aligned}$$

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 jth 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

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

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

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

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

(Λ_j being the eigenvalues of $\operatorname{Hess}_{x_0} \phi$*).*

Note: No "$+\,O(y^3)$". Cf.
mean value theorem $\quad f(x) = f(0) + f'(c)x$
vs. Taylor's theorem $\quad f(x) = f(0) + f'(0)x + O(x^2)$.

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 $M \mapsto M^{\mathrm{t}}\bigl(\operatorname{Hess}_{x_0} \phi\bigr)M$ to write $H(x) = M(H(x))^{\mathrm{t}}\bigl(\operatorname{Hess}_{x_0} \phi\bigr)M(H(x))$ and hence $y \equiv M(H(x))(x - x_0)$.

$$I(t) \equiv \int_{\mathbf{R}^n} e^{it\phi(x)} a(x)\,dx, \qquad \nabla\phi(x_0) = 0.$$

Put together the three theorems to get:

Stationary Phase Theorem. *Assume* $\phi \in C^\infty_{\mathbf{R}}(\mathbf{R}^n)$, $a \in C^\infty_0(\mathbf{R}^n)$, *and the only critical points of* ϕ *in some neighborhood of* $\operatorname{supp} a$ *are nondegenerate (and hence isolated); call them* $x_{01}, \ldots, x_{0K}$. *Then as* $t \to \infty$

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

where b_j^k *are certain PDOs and* σ_k *is the signature of* $\operatorname{Hess}_{x_{0k}} \phi$.

See (for instance) S. Zelditch, `math.SP/0111078`, for a Feynman-diagram algorithm for b_j^k.

Remark: Often in practice the critical points are not isolated. Instead, there may be a whole submanifold $\mathcal{T}$ of critical points, with $\operatorname{Hess}\phi$ 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 $H(\mathbf{x}, \mathbf{p})$ be a (smooth) real-valued function defined on [a subset of, or manifold like] $\mathbf{R}^{2d}$ (*phase space*). Usually, H is a second-degree polynomial in $\mathbf{p}$. Main example:

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

Then

$$\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}}, \qquad \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{x}}$$

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

$$\bigl(\mathbf{x}(t), \mathbf{p}(t)\bigr) = \Phi_t(\mathbf{x}_0, \mathbf{p}_0)$$

for initial data $\bigl(\mathbf{x}(t), \mathbf{p}(t)\bigr) = (\mathbf{x}_0, \mathbf{p}_0)$.
All this is equivalent to a Newtonian equation of motion (second-order ODE for $\mathbf{x}$) plus a definition of $\mathbf{p}$ in terms of $\dot{\mathbf{x}}$ (or vice versa).

Energy is conserved:

$$\frac{d}{dt} H\bigl(\mathbf{x}(t), \mathbf{p}(t)\bigr) = \frac{\partial H}{\partial \mathbf{x}} \frac{d\mathbf{x}}{dt} + \frac{\partial H}{\partial \mathbf{p}} \frac{d\mathbf{p}}{dt} = 0.$$

So $H\bigl(\mathbf{x}(t), \mathbf{p}(t)\bigr) \equiv E$.

Two PDEs associated with H

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

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

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

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

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

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

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

$$0 \doteq A\left[\frac{\partial S}{\partial t} + \frac{1}{2m}\,|\nabla S|^2 + V\right] - i\hbar\left[\frac{\partial A}{\partial t} + \frac{1}{m}\nabla A\cdot\nabla S + \frac{1}{2m}\,A\nabla^2 S\right] - \frac{\hbar^2}{2m}\nabla^2 A.$$

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,

$$-\frac{\partial S(t,\mathbf{x})}{\partial t} = H\big(\mathbf{x}, \nabla S(t,\mathbf{x})\big),$$

and a (local) curve $\mathbf{x}(t)$ satisfying

$$\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}}\Big(\mathbf{x}(t), \nabla S\big(t,\mathbf{x}(t)\big)\Big) \doteq \frac{1}{m}\nabla S\big(t,\mathbf{x}(t)\big).$$

Then $\Big(\mathbf{x}(t), \nabla S\big(t,\mathbf{x}(t)\big)\Big)$ is a trajectory of the Hamiltonian flow (with $\mathbf{p}(t) = \nabla S\big(t,\mathbf{x}(t)\big)$).

Proof: $\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}}$ is satisfied by assumption. Why $\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{x}}$? 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: $\quad \dfrac{dp_i}{dt} = -\,\dfrac{\partial H}{\partial x_i}\,.$

Corollary: Entrance of the *Lagrangian*.

$$\frac{d}{dt}S\big(t,\mathbf{x}(t)\big) = \frac{\partial S}{\partial t} + \dot{\mathbf{x}}\cdot\nabla S = -H + \dot{\mathbf{x}}\cdot\mathbf{p} \equiv L\big(\mathbf{x}(t), \dot{\mathbf{x}}(t)\big).$$

(2) Conversely, assume we know the flow Φ_t. The previous corollary suggests that we should get solutions of HJ by integrating L along the trajectories. Indeed, for given $(t, \mathbf{x}, \mathbf{x}_0)$ in a sufficiently small neighborhood in $\mathbf{R}^{1+2d}$, the *two-point boundary problem*

$$\mathbf{x}(0) = \mathbf{x}_0\,, \quad \mathbf{x}(t) = \mathbf{x}$$

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

$$S(t, \mathbf{x}; \mathbf{x}_0) = \int_0^t L\bigl(\mathbf{x}(u), \dot{\mathbf{x}}(u)\bigr)\, du.$$

Then S solves HJ. (Note that arbitrary initial data $S_0(\mathbf{x}_0)$ could be added.)

PROOF: is somewhat complicated. See

- Arnold, *Mathematical Methods of Classical Mechanics*, pp. 253–258 with pp. 233–237.
- Molzahn et al., *Ann. Phys.* (NY) **214** (1992), Appendix A.

Corollary: Initial and final momenta.

$$\mathbf{p}(t) = \nabla_{\mathbf{x}} S(t, \mathbf{x}; \mathbf{x}_0).$$

By symmetry,

$$\mathbf{p}(0) = -\nabla_{\mathbf{x}_0} S(t, \mathbf{x}; \mathbf{x}_0) \qquad [\,+\nabla S_0(\mathbf{x}_0), \text{in general}].$$

(3) Return to (1) and assume we have a parametrized family of (local) solutions of HJ, $S(t,\mathbf{x};\mathbf{p}_0)$, such that $S(0,\mathbf{x};\mathbf{p}_0)=\mathbf{x}\cdot\mathbf{p}_0$. Then *any* flow trajectory, $\bigl(\mathbf{x}(t),\mathbf{p}(t)\bigr)$, running through the domain of S is of the form described in (1), with $\mathbf{p}(0)=\mathbf{p}_0$.

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

$$\frac{d\tilde{\mathbf{x}}(t)}{dt}=\frac{\partial H}{\partial \mathbf{p}}\Bigl(\tilde{\mathbf{x}}(t),\nabla S\bigl(t,\tilde{\mathbf{x}}(t);\mathbf{p}(0)\bigr)\Bigr),\quad \tilde{\mathbf{x}}(0)=\mathbf{x}(0),$$

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

Remark: In the context of (2), these solutions are those with $S_0(\mathbf{x}_0)=\mathbf{x}_0\cdot\mathbf{p}_0$. It follows that

$$\begin{aligned}\mathbf{p}(0)&=-\nabla_{\mathbf{x}_0}S(t,\mathbf{x};\mathbf{p}_0)+\nabla S_0(\mathbf{x}_0)\\&=-\nabla_{\mathbf{x}_0}S(t,\mathbf{x};\mathbf{p}_0)+\mathbf{p}_0\,,\end{aligned}$$

but we know $\mathbf{p}(0)=\mathbf{p}_0$, so $\nabla_{\mathbf{x}_0}S(t,\mathbf{x};\mathbf{p}_0)=0$, as the notation implies.

(4) Let's be more precise about the two-point boundary problem. We have a flow

$$\Phi_t(\mathbf{x}_0, \mathbf{p}_0) = (\mathbf{x}, \mathbf{p}) \equiv \bigl(\mathbf{x}(t, \mathbf{x}_0, \mathbf{p}_0), \mathbf{p}(t, \mathbf{x}_0, \mathbf{p}_0)\bigr).$$

Assume that for each $(t, \mathbf{p}_0)$ in some open set the map $\mathbf{x}_0 \mapsto \mathbf{x}(t, \mathbf{x}_0, \mathbf{p}_0)$ is a diffeomorphism, so it has inverse $\mathbf{x} \mapsto \mathbf{x}_0(t, \mathbf{x}, \mathbf{p}_0)$. In words, $\mathbf{x}_0$ is the initial position of a particle of initial momentum $\mathbf{p}_0$ that at time t arrives at $\mathbf{x}$. (In (2) the roles of $\mathbf{x}_0$ and $\mathbf{p}_0$ were interchanged.) We now claim

$$\mathbf{x}_0(t, \mathbf{x}, \mathbf{p}_0) = \nabla_{\mathbf{p}_0} S(t, \mathbf{x}; \mathbf{p}_0).$$

Proof: Write the claim as

$$\mathbf{x}_0(t, \mathbf{x}, \mathbf{p}_0) = \nabla_{\mathbf{p}_0} S\bigl(t, \mathbf{x}(t, \mathbf{x}_0, \mathbf{p}_0); \mathbf{p}_0\bigr).$$

It holds at $t = 0$:

$$\nabla_{\mathbf{p}_0} S(0, \mathbf{x}(0); \mathbf{p}_0) = \nabla_{\mathbf{p}_0} [\mathbf{x}_0 \cdot \mathbf{p}_0] = \mathbf{x}_0 \,.$$

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

$$\frac{dx_{0i}}{dt} = \frac{\partial^2 S}{\partial t\, \partial p_i} + \sum_j \frac{\partial^2 S}{\partial x_j\, \partial p_i} \frac{dx_j}{dt} \,,$$

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

$S(t,\mathbf{x};\mathbf{x}_0) = \int_0^t L$ satisfies

$$\mathbf{p} = \nabla_{\mathbf{x}} S(t,\mathbf{x};\mathbf{x}_0), \quad \mathbf{p}_0 = -\nabla_{\mathbf{x}_0} S(t,\mathbf{x};\mathbf{x}_0).$$

In the language of Goldstein, *Classical Mechanics*, $-S(t,\mathbf{x},;\mathbf{x}_0)$ is a *generating function of type* F_1 for Φ_t regarded as a *canonical transformation* from the old variables $(\mathbf{x}_0,\mathbf{p}_0)$ to the new variables $(\mathbf{x},\mathbf{p})$.

$S(t,\mathbf{x};\mathbf{p}_0) = \int_0^t L + \mathbf{x}_0 \cdot \mathbf{p}_0$ (which is actually independent of $\mathbf{x}_0$ and has initial data $S(0,\mathbf{x};\mathbf{p}_0) = \mathbf{x}\cdot\mathbf{p}_0$) satisfies

$$\mathbf{p} = \nabla_{\mathbf{x}} S(t,\mathbf{x};\mathbf{p}_0), \quad \mathbf{x}_0 = \nabla_{\mathbf{p}_0} S(t,\mathbf{x};\mathbf{p}_0).$$

So $-S(t,\mathbf{x};\mathbf{p}_0)$ is a *generating function of type* F_3 for Φ_t .

Remark: Therefore, contrary to appearance, $S(t,\mathbf{x};\mathbf{x}_0)$ does not approach 0 as $t \to 0$ if $\mathbf{x} \neq \mathbf{x}_0$. The reason is that if the particle gets from $\mathbf{x}_0$ to $\mathbf{x}$ in a very short time, then L is very large!

$$S(0,\mathbf{x};\mathbf{x}_0) = (\mathbf{x}-\mathbf{x}_0)\cdot\mathbf{p}_0 \,.$$

The transport equation

Recall that to solve the Schrödinger equation (for $H = \frac{\mathbf{p}^2}{2m} + V$) 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

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

Therefore,

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

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

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

(where $\mathbf{x}(0) = \mathbf{x}_0$, $\mathbf{x}(t) = \mathbf{x}$). Higher-order terms $\hbar^n A_n$ can be calculated in the same way.

Alternative solution: *Van Vleck determinant.*

$$A_0(\mathbf{x}) = \sqrt{|\det \nabla_{\mathbf{x}} \nabla_{\mathbf{x}_0} S|}\,.$$

This determinant becomes infinite at places $\mathbf{x}$ where the flow ceases to be a diffeomorphism (trajectories emerging from $\mathbf{x}_0$ intersect for the first time).