The Uniform Semi-Classical Approximation

$$I(\alpha) = \int d^N x \exp\left[if(\boldsymbol{x};\alpha)\right]$$

which depends on a parameter α and, for each α, $f(\boldsymbol{x};\alpha)$ has *at most two stationary points* $\boldsymbol{x}^{(1)}(\alpha)$ and $\boldsymbol{x}^{(2)}(\alpha)$:

$$\nabla f(\boldsymbol{x};\alpha) = 0 \qquad \text{for } \boldsymbol{x} = \boldsymbol{x}^{(1)}(\alpha),\ \boldsymbol{x}^{(2)}(\alpha).$$

$\boldsymbol{x}^{(1)}(\alpha)$ and $\boldsymbol{x}^{(2)}(\alpha)$ coalesce when $\alpha = \bar{\alpha}$.

The uniform asymptotic evaluation of (1.10) consists of the following steps.

1) Find the most simple function $\psi_0(y;\beta)$ which depends on a single parameter β, and which has at most two stationary points that coalesce at $\beta = \bar{\beta}$. In the present case,

$$\begin{cases} \psi_0(y;\beta) = \frac{1}{3}y^3 - \beta y\,, \\ y^{(1)} = \beta^{\frac{1}{2}}\,, \qquad y^{(2)} = -\beta^{\frac{1}{2}}\,, \\ \bar{\beta} = 0\,. \end{cases}$$

2) Extend the «generic» function $\psi_0(y;\beta)$ to N dimensions without affecting its stationary-point structure. This is done by constructing

$$\begin{cases} \varphi(\boldsymbol{y};\beta) = \psi_0(y_1;\beta) + \frac{1}{2}\sum_{i=2}^{N} y_i^2\,, \\ \nabla\varphi(\boldsymbol{y};\beta) = 0 \Rightarrow \begin{cases} \boldsymbol{y}^{(1)}(\beta) = (\beta^{\frac{1}{2}}, 0, \ldots, 0)\,, \\ \boldsymbol{y}^{(2)}(\beta) = (-\beta^{\frac{1}{2}}, 0, \ldots, 0)\,. \end{cases} \end{cases}$$

The uniform approximation to $I(\alpha)$ will be expressed in terms of the integrals

$$I_0(\beta) = \int \mathrm{d}\eta \exp[i\psi_0(\eta;\beta)]\,,$$

$$I_1(\beta) = -\frac{\partial I_0}{\partial\beta} = -i\int \mathrm{d}\eta \frac{\partial\psi_0}{\partial\beta} \exp[i\psi_0(\eta;\beta)]\,,$$

which in this case are expressed in terms of the Airy function and its derivative.

3) Change the integration variables $\boldsymbol{x}$ to $\boldsymbol{y}$ through a mapping which preserves the relation

$$f(\boldsymbol{x};\alpha) = \varphi(\boldsymbol{y};\beta) + A\,.$$

Such a mapping is one to one only if the stationary points of φ are mapped onto those of f through (1.15). Imposing this condition on the mapping, we obtain from (1.13) and (1.15) as many relations as needed to determine A and β for every value of α:

$$\begin{cases} f^{(1)} = f(\boldsymbol{x}^{(1)};\alpha) = -\frac{2}{3}\beta^{\frac{3}{2}} + A\,, \\ f^{(2)} = f(\boldsymbol{x}^{(2)};\alpha) = \frac{2}{3}\beta^{\frac{3}{2}} + A\,. \end{cases}$$

$$A = \tfrac{1}{2}(f^{(1)} + f^{(2)})\,, \qquad \beta = [\tfrac{3}{4}(f^{(2)} - f^{(1)})]^{\frac{2}{3}}\,.$$

The integral (1.10) in terms of the new integration variables now reads

$$I(\alpha) = \int \mathrm{d}^N y\, G(\boldsymbol{y}) \exp[i(\varphi(\boldsymbol{y};\beta) + A)]$$

and the complexity of the integration now resides in the Jacobian determinant $G(\boldsymbol{y}) = \partial(x_1 \dots x_N)/\partial(y_1 \dots y_N)$.

4) Approximate $G(\boldsymbol{y})$ in such a manner that at the stationary points the approximation and the original $G(\boldsymbol{y})$ coincide. This is done by writing

$$G(\boldsymbol{y}) \simeq g_0(\beta) + g_1(\beta)\,\frac{\partial\varphi(\boldsymbol{y};\beta)}{\partial\beta}\,. \tag{1.18}$$

The $\boldsymbol{y}$-independent g_0 and g_1 are determined by requiring

$$G(\boldsymbol{y}^{(i)}) = g_0(\beta) + g_1(\beta)\,\frac{\partial\varphi(\boldsymbol{y}^{(i)};\beta)}{\partial\beta}\,, \qquad i = 1, 2\,. \tag{1.19}$$

At the stationary points,

$$\left\{\begin{aligned} &G(\boldsymbol{y}^{(i)}) = \frac{\partial(x_1 \dots x_N)}{\partial(y_1 \dots y_N)} = \left[\frac{\det\left(\dfrac{\partial^2 f}{\partial x_m\,\partial x_n}\right)^{(i)}}{\det\left(\dfrac{\partial^2\varphi}{\partial y_m\,\partial y_n}\right)^{(i)}}\right]^{-\frac{1}{2}},\\ &\det\left(\frac{\partial^2\varphi}{\partial y_m\,\partial y_n}\right)^{(i)} = 2\,(\pm\beta^{\frac{1}{2}})\,, \end{aligned}\right. \tag{1.20}$$

with this information g_0 and g_1 can be easily determined. Substituting (1.18) in (1.17), we see that the y_1-integration yields a linear combination of the functions I_0 and I_1 (eq. (1.14)) with the corresponding coefficients g_0 and g_1. The $y_2 \dots y_N$ integration is trivial and brings about an overall factor. The final expression for the uniform approximation for the example which was discussed here is

$$I(\alpha) \simeq (2\pi)^{N/2}\left\{\frac{1}{\Delta(1)^{\frac{1}{2}}}\,Bi^{(-)}(-Z)\exp\left[if^{(1)} + \frac{i\pi}{4}\,\bar{\nu}^{(1)}\right] + \right.$$
$$\left. + \frac{1}{\Delta(2)^{\frac{1}{2}}}\,Bi^{(+)}(-Z)\exp\left[if^{(2)} + \frac{i\pi}{4}\,\bar{\nu}^{(2)}\right]\right\}. \tag{1.21}$$

$f^{(i)}$ were already defined in (1.16) as the values of $f(\boldsymbol{x};\alpha)$ at the stationary points,

$$(1.21a)\quad \begin{cases} Z=\frac{3}{4}(f^{(1)}-f^{(2)}) & \text{(see eq. (1.16))}\,, \\ Bi^{(\pm)}(-Z)=\pi^{\frac{1}{2}}[Z^{\frac{1}{4}}\,\mathrm{Ai}\,(-Z)\pm iZ^{-\frac{1}{4}}\,\mathrm{Ai}\,(-Z)]\exp\left[\mp i\left(\frac{2}{3}Z^{\frac{3}{2}}-\frac{\pi}{4}\right)\right], \\ \Delta(i)=\left[\det\left(\frac{\partial^2 f}{\partial x_i\,\partial x_j}\right)\right]_{\boldsymbol{x}=\boldsymbol{x}^{(i)}}, & i=1,2\,, \end{cases}$$

and $\nu^{(i)}$ stand for the signature (the difference in the number of positive and negative eigenvalues) of the quadratic form whose determinant is $\Delta(i)$.

1) *The Airy uniform approximation.* Consider the transition amplitude (*) for situations in which only two stationary paths (= classical trajectories) correspond to the transition $\boldsymbol{x}_1\to\boldsymbol{x}_2$ at time T. Considering the path integral as a N-dimensional Riemann integral, we can use the result (1.21) to express it in terms of Airy functions. When we let $N\to\infty$, the various parameters in (1.21) obtain the following values:

$f^{(i)}=S^{(i)}_{\mathrm{cl}}$, the classical actions along the i (= 1, 2) trajectory,

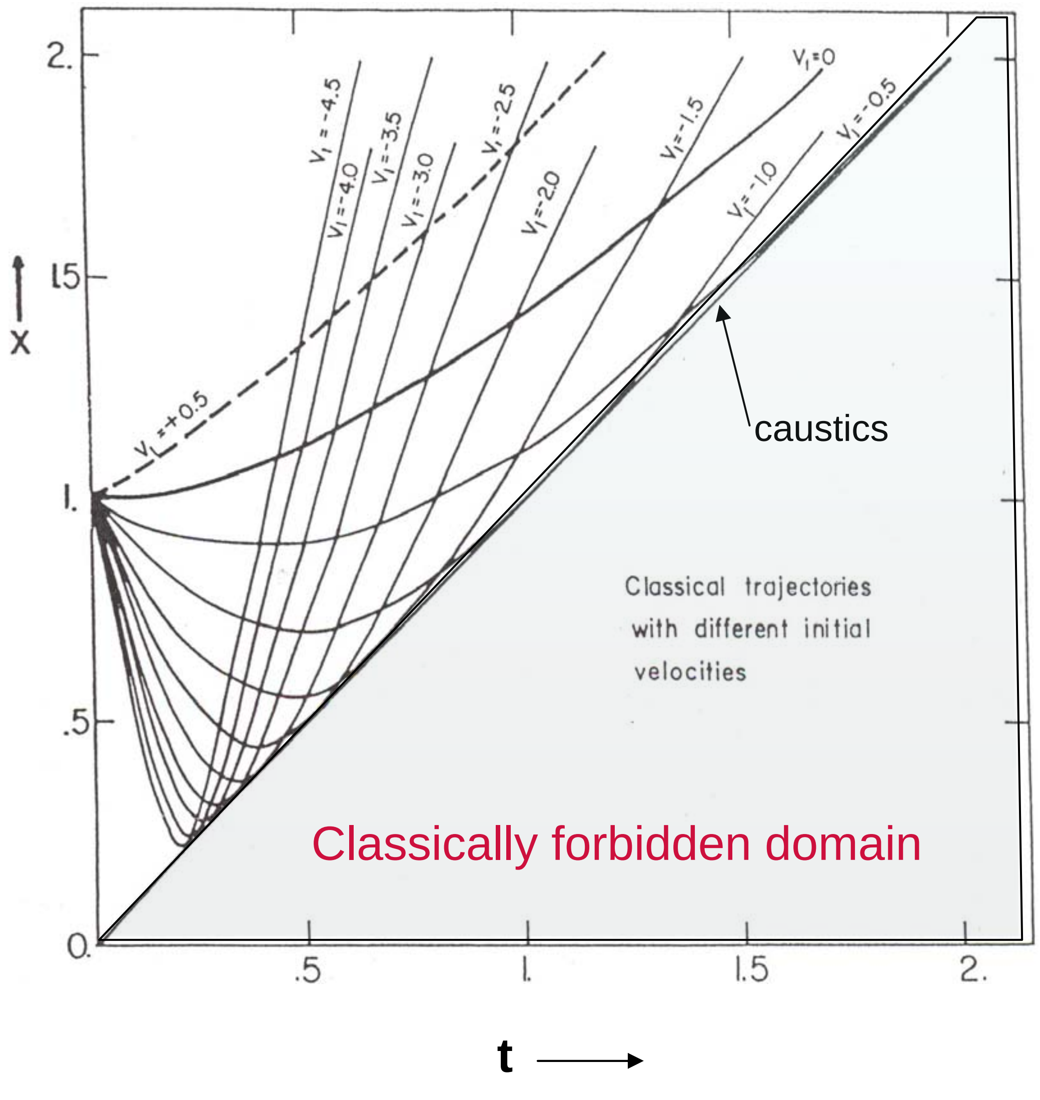
$$\Delta(i)=\det\left(\frac{\partial^2 S_{\mathrm{cl}}}{\partial x_i(0)\,\partial x_j(T)}\right)^{(i)}=\det\left(\frac{\partial x_i(T)}{\partial p_j(0)}\right)^{(i)},$$

$\nu^{(i)}$ as in the primitive expression

$$(*)\qquad K_{scl}(\mathbf{q}''t'';\mathbf{q}'t') \;=\; \left(\frac{1}{2\pi i\hbar}\right)^{\frac{f}{2}}\sum_{cl=1}^{2}\frac{\exp i\left(\frac{S_{cl}}{\hbar}-\frac{\pi}{2}\nu_{cl}\right)}{\left|\det\frac{\partial q_j(t'')}{\partial p_k(t')}\right|_{cl}^{\frac{1}{2}}}$$

The summation is over the two classical trajectories which satisfy the boundary conditions $\mathbf{q}(t')=\mathbf{q}'$; $\mathbf{q}(t'')=\mathbf{q}''$.

Application I: The Uniform approximation for the problem:



II.5 Simple Illustration - Motion in a $1/x^2$ Potential

We treat the one-dimensional problem in which a particle of mass m moves in a potential of the form

$$V(x) = \frac{\hbar^2}{2m} \frac{\kappa^2}{x^2} \tag{2.81}$$

κ^2 is a positive dimensionless constant. We wish to calculate the propagator for the motion of the particle from $x=x_1$ at $t=0$ to $x=x_2$ at $t=T$.

The classical trajectories which start at $x=x_1$ can be explicitly expressed as

$$x^2(t, v_1) = (x_1+tv_1)^2 + x_c^2 \quad . \tag{2.82}$$

Here v_1 is the initial velocity at $t=0$ and

$$x_c = \frac{\hbar}{m} \kappa \cdot t/x_1 \quad . \tag{2.83}$$

The classical trajectories are shown in Fig.2 for a few values of the initial velocities. The (x,t) plane is clearly divided into classically accessible and classically inaccessible regions. The dividing line is the caustic

$$\partial x(t, v_1)/\partial v_1 = 0 \tag{2.84}$$

which can be solved explicitly to give

$$x = \frac{\hbar}{m} \kappa \ t/x_1 = x_c \ . \tag{2.85}$$

Given a point (x_2,T), one can solve (2.82) to find two classical trajectories which are characterized by different initial velocities. As long as (x_2,T) is classically accessible, the two solutions $v_1^{(+)}$ and $v_1^{(-)}$ are real. One of the trajectories is reflected from the caustic and its index is $\nu^{(-)}=1$. The other does not touch the caustic and its index is $\nu^{(+)}=0$. The trajectories coalesce as (x_2,T) approach the caustic and when (x_2,T) enters the forbidden region, the velocities $v_1^{(+)}$ and $v_1^{(-)}$, as well as the trajectories, become complex conjugate pairs. The classical complex trajectories have complex values at all times except the initial and final times. Therefore, the complex trajectories avoid the caustic.

The structure of the complex and real classical trajectories indicate that there are only two saddle points to the path integral which defines the propagator. The catastrophe which occurs when the saddle points coincide can be treated by the Airy uniform approximation derived above.

Let

$$r_i^2 = \frac{mx_i^2}{\hbar T} \qquad i = 1,2$$

$$b = \left(\frac{\hbar T}{m}\right)^{\frac{1}{2}} \tag{2.86}$$

and

$$R = \left(\frac{r_1^2 r_2^2}{\kappa^2} - 1\right)^{\frac{1}{2}} \qquad \text{real trajectories} \tag{2.87a}$$

$$\rho = \left(1 - \frac{r_1^2 r_2^2}{\kappa^2}\right)^{\frac{1}{2}} \qquad \text{complex trajectories} \tag{2.87b}$$

The action integrals for the real and complex trajectories are easily found

$$\frac{1}{\hbar} S^{(\pm)} = \frac{1}{2}(r_1^2 + r_2^2) \mp \kappa [R + \text{arctg}(1/R) - \frac{(1 \mp 1)\pi}{2}] \tag{2.88a}$$

$$\frac{1}{\hbar} S^{(\pm)} = \frac{1}{2}(r_1^2 + r_2^2) - \kappa\pi/2 \mp i\kappa [\rho + \text{argth}\rho] \tag{2.88b}$$

The expression for the Van Vleck determinants are

$$\left[\frac{\partial x(T)}{\partial v_1}\right]^{\pm} = \pm\, T \, \frac{\kappa}{r_1 r_2}\, R \tag{2.89a}$$

$$\left[\frac{\partial x(T)}{\partial v_1}\right]^{\pm} = \pm\, i\, T \, \frac{\kappa}{r_1 r_2} \cdot \rho \quad . \tag{2.89b}$$

These results can now be substituted in the uniform expression (2.69) and after some simple algebra we obtain

$$K_{\kappa}^{\mathrm{UNIFORM}}(x_2,T;\, x_1,0) = i^{-(\kappa+1)}\, \sqrt{2}\, b^{-1} \left(\frac{r_1 r_2}{\kappa R}\right)^{\frac{1}{2}} \times$$
$$\times\ \zeta^{1/4} \mathrm{Ai}(-\zeta) \exp[\tfrac{i}{2}(r_1^2 + r_2^{\,2})] \tag{2.90}$$

with

$$\zeta = \left\{\frac{3\kappa}{2}\,(R + \mathrm{arctg}\, R^{-1} - \frac{\pi}{2})\right\}^{2/3} \tag{2.91}$$

The accuracy of the expression (2.90) can be checked by comparing it to the exact result which is most easily derived from the partial wave expansion of the free propagator in three dimensions

$$K_{\ell}^{Q.M.} = i^{-(\ell+3/2)}(r_1 r_2)^{\frac{1}{2}} \exp[\tfrac{i}{2}(r_1^2 + r_2^2)] \times \qquad (2.92)$$

$$\times \quad J_{\ell+\frac{1}{2}}(r_1 r_2)$$

where $J_{\ell+\frac{1}{2}}$ is the regular Bessel function and ℓ is a positive integer. The condition that a point (x_2,T) be forbidden can be written as

$$r_1 r_2/\kappa < 1.$$

The argument of the Bessel function in (2.92) is therefore less than $\ell+\frac{1}{2}$ and the absolute value of the propagator vanishes as $r_1 r_2 \to 0$.

For allowed transitions, $r_1 r_2 > \ell+\frac{1}{2}$ and the Bessel function displays an oscillatory behavior which can be interpreted as the result of the interfering contributions which come from the two allowed trajectories. Putting $\kappa = (\ell(\ell+1))^{\frac{1}{2}} \cong \ell+\frac{1}{2}$ for large values of κ one can relate the expressions for $K_\ell^{Q.M.}$ and $K_\kappa^{UNIFORM}$ using [90]

$$J_\kappa(\kappa y) = \frac{2\sqrt{\pi}}{\Gamma(\kappa+1)} \kappa^{\kappa+1/6} e^{-\kappa} \left(\frac{y^2-1}{\eta}\right)^{-1/4} Ai(-\kappa^{2/3}\eta)[1+0(\kappa^{-1})],$$

$$\frac{2}{3}\eta^{3/2} = (y^2-1)^{\frac{1}{2}} - \arccos(y^{-1}), \quad (1 \leq y < \infty). \tag{2.93}$$

This relation is uniform in y and using it in (2.92) one obtains the expression (2.90) for $K_\kappa^{UNIFORM}$ up to the term of the order κ^{-1}. This is of course the expected accuracy of a semi-classical approximation.

Application II: The initial value representation

For any given initially condition $\boldsymbol{x}_1$, we solve the classical equations of motion by specifying the initial momenta $\boldsymbol{p}(0)$. The trajectories become a function of the initial momenta, and the action integral along the trajectory can also be considered as a function of $\boldsymbol{p}(0)$, to be denoted by $S_{cl}(\boldsymbol{p}(0))$. Consider the function

$$\Phi(\boldsymbol{p}(0)) = S_{cl}(\boldsymbol{p}(0)) - \sum_{i=1}^{M} [x_i^T(\boldsymbol{p}(0)) - x_i^{(2)}]\, p_i^T(\boldsymbol{p}(0)) \,. \tag{1.22}$$

Here, $x_i^T(\boldsymbol{p}(0))$ and $p_i^T(\boldsymbol{p}(0))$ are the values of the i-th components of the position and momentum vectors at the time $t = T$. They are calculated for the classical trajectory which is specified by the initial momentum vector $\boldsymbol{p}(0)$. $x_i^{(2)}$ are the components of the vector $\boldsymbol{x}_2$: the boundary condition for the transition.

The stationary points of $\Phi\,(\boldsymbol{p}(0))$ can be easily calculated. Since $\partial S_{cl}/\partial p_j(0) = \sum_i p_i^T(\partial x_i^T/\partial p_j(0))$,

$$\frac{\partial \Phi}{\partial p_j(0)} = -\sum_{i=1}^{M} \left(x_i^T(\boldsymbol{p}(0)) - x_i^{(2)}\right) \frac{\partial p_i^T(\boldsymbol{p}(0))}{\partial p_j(0)} \,. \tag{1.23}$$

So that, if $\det\left(\partial p_i^T(\boldsymbol{p}(0))/\partial p_j(0)\right) \neq 0$, the stationary points of Φ fulfil the requirement

$$\boldsymbol{x}^T(\boldsymbol{p}(0)) = \boldsymbol{x}_2 \,. \tag{1.24}$$

That is, for each classical trajectory which satisfies the boundary condition (1.24), we assign the initial momentum vector $\boldsymbol{p}(0)$ at the stationary point of Φ. Φ has, therefore, the same number of stationary points as the action functional, and can be used as a mapping function in a uniform approximation. Carrying out the mapping procedure as indicated above, one finally obtains

$$K(\boldsymbol{x}_1, \boldsymbol{x}_2; T) \simeq \int \mathrm{d}^M p(0) \left| \det\left(\frac{\partial p_i^T(\boldsymbol{p}(0))}{\partial p_j(0)}\right)\right|^{\frac{1}{2}} \exp\left[i/\hbar\, \Phi(\boldsymbol{p}(0))\right] . \tag{1.25}$$

Application III: Transmission through a barrier (inverted harmonic oscillator)

The propagtor across an **inverted** harmonic oscillator $V(x) = -\frac{1}{2}m\omega^2 q^2$:

$$K_{scl}(q''T; q'0) = \frac{1}{2\pi i\hbar}\left(\frac{m\omega}{\sinh \omega T}\right)^{\frac{1}{2}} \exp i\left[\frac{m\omega}{2\hbar \sinh \omega T}\left(\cosh \omega T(q''^2 + q'^2) - 2q'q''\right)\right]$$

Transmission is defined at a **constant energy**:

$$G(q'', q'; E) = \frac{1}{i\hbar}\int_0^\infty \mathrm{d}T K_{scl}(q''T; q'0)\mathrm{e}^{\frac{i}{\hbar}ET}$$

The T integration is taken in the SPA. SP condition:

$$E - \frac{m\omega^2}{2\sinh^2 \omega T}\left[(q'' - q')^2 - 2q'q'' \cosh \omega T\right] = 0$$

$E > 0$: (**Classically allowed** transitions)

$$T = T_0 - i\ 2n\pi/\omega\ ;\ n = 0, 1, 2, ...$$

$E < 0$: (**Classically forbidden** transitions)

$$T = T_0 - i\ (2n + 1)\pi/\omega\ ;\ n = 0, 1, 2, ...$$

Equi-spaced saddle points:

$E > 0$: (**Classically allowed** transitions)

$$T = T_0 - i\ 2n\pi/\omega\ ;\ n = 0, 1, 2, ...$$

$E < 0$: (**Classically forbidden** transitions)

$$T = T_0 - i\ (2n+1)\pi/\omega\ ;\ n = 0, 1, 2, ...$$

Note: as $E \to 0$

$$\Delta T = \left(\frac{\partial^2 S_{cl}}{\partial T^2}\right)^{-\frac{1}{2}} \approx \left(\frac{\hbar}{\omega|E|}\right)^{-\frac{1}{2}}$$

Uniform approximation: $\phi_0(y, \beta) = \exp(-y) - \beta y$

$$\beta < 0\quad :\quad T = -\log\beta - i\ 2n\pi/\omega\ ;\ n = 0, 1, 2, ...$$

$$\beta > 0\quad :\quad T = -log\beta - i\ (2n+1)\pi/\omega\ ;\ n = 0, 1, 2, ...$$

$$I_0(\beta) = \int_{-\infty}^{\infty} \mathrm{d}y \exp\left[i\mathrm{e}^{-y} - (1/2 + i\beta)y\right] = \exp\left[\frac{1}{4}i\pi - \frac{1}{2}\pi\beta\right]\Gamma(\frac{1}{2} + i\beta)$$

Following the Uniform way, and mapping : $\beta = -\frac{E}{\hbar\omega}$

$$\boxed{P(E) = |G(E)|^2 = \frac{\exp(-\pi\beta)}{2\pi}|\Gamma(\frac{1}{2} + i\beta)|^2 = \frac{1}{1 + \mathrm{e}^{2\pi\beta}}}$$

End of section II