Multiple Groenewold Products:

from path integrals
to semiclassical correlations

1. Translation and reflection bases for operators

Translation operators,

$$\hat{T}_{\boldsymbol{\xi}} = \exp\{\frac{i}{\hbar}(\boldsymbol{\xi} \wedge \hat{\mathbf{x}})\}$$

correspond to classical translations, $\mathbf{x}_0 \mapsto \mathbf{x}_0 + \boldsymbol{\xi}$
within the classical phase space, $\{\mathbf{x} = (\mathbf{p}, \mathbf{q})\}$

They form a complete operator basis, so that any operator

$$\hat{A} = \frac{1}{(2\pi\hbar)^N} \int d\boldsymbol{\xi}\ \tilde{A}(\boldsymbol{\xi})\ \hat{T}_{\boldsymbol{\xi}}$$

with the expansion coefficients:

$$\tilde{A}(\boldsymbol{\xi}) = \mathrm{tr}\ (\hat{T}_{-\boldsymbol{\xi}}\ \hat{A}).$$

This is the ***chord symbol*** *of the operator* $\hat{A}$.

The Fourier transform of the translation operators defines unitary ***reflection operators***,

$$2^N \hat{R}_{\mathbf{x}} = \frac{1}{(2\pi\hbar)^N} \int d\boldsymbol{\xi} \, \exp\{\frac{i}{\hbar}(\mathbf{x} \wedge \boldsymbol{\xi})\} \, \hat{T}_{\boldsymbol{\xi}},$$

corresponding to the classical reflections, $\mathbf{x}_0 \mapsto 2\mathbf{x} - \mathbf{x}_0$.

An arbitrary operator, $\hat{A}$, can be decomposed in this basis:

$$\hat{A} = 2^N \int \frac{d\mathbf{x}}{(2\pi\hbar)^N} \, A(\mathbf{x}) \, \hat{R}_{\mathbf{x}}$$

such that the expansion coefficient

$$A(\mathbf{x}) = 2^N \mathrm{tr} \, \left[\hat{R}_{\mathbf{x}} \, \hat{A}\right]$$

is the ***Weyl-Wigner symbol*** for $\hat{A}$.

In the case of the density operator,

$$\hat{\rho} = 2^N \int d\mathbf{x} \, W(\mathbf{x}) \, \hat{R}_{\mathbf{x}}$$

W(x) *is just the **Wigner function***.

Grossmann
Royer

The chord symbol for a product of operators, $\hat{A}_n \hat{A}_n \ldots \hat{A}_1$,

$$\widetilde{A}_n \widetilde{A}_{n-1} \ldots \widetilde{A}_1(\xi) = \int \frac{d\xi_n \ldots d\xi_1}{(2\pi\hbar)^{nN}} \widetilde{A}_n(\xi_n) \ldots \widetilde{A}_1(\xi_1) \ \mathrm{tr}\, \hat{T}_{-\xi} \hat{T}_{\xi_n} \ldots \hat{T}_{\xi_1}$$

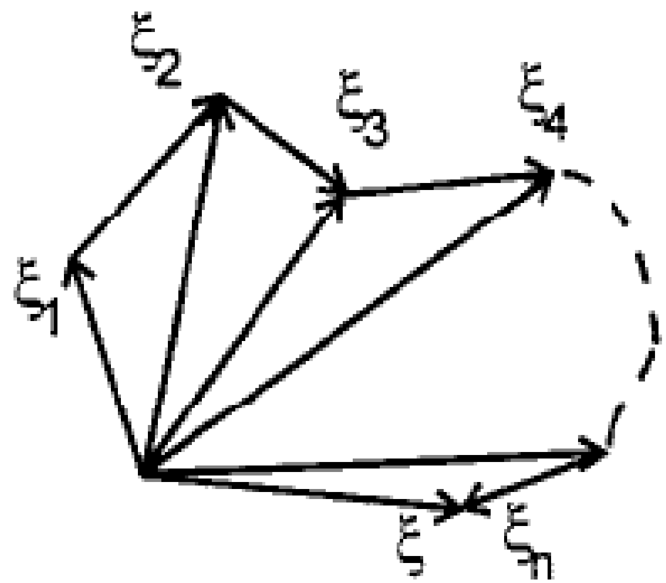
is determined by the ***quantum translation group:***

$$\hat{T}_{\xi_n} \hat{T}_{\xi_{n-1}} \ldots \hat{T}_{\xi_1} = \hat{T}_{\xi_1 + \ldots + \xi_n} \exp\left[\frac{-i}{\hbar} D_{n+1}(\xi_1, \ldots, \xi_n)\right].$$

The final translation operator corresponds to the overall classical translation and $D_{n+1}(\xi_1, \ldots, \xi_n)$ is the symplectic area of the $(n+1)$-sided polygon formed by the n translations.

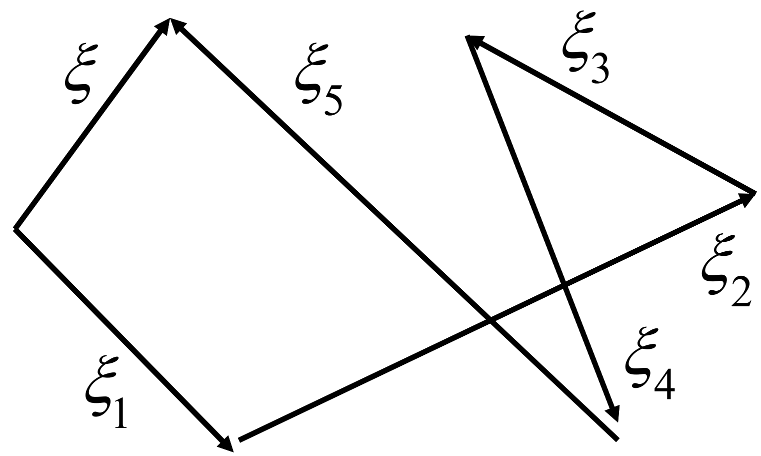
Tecelating the polygon with triangles, specifies

$$D_{n+1}(\xi_1,\ldots,\xi_n)=\frac{1}{2}[\xi_1\wedge\xi_2+\ldots+(\xi_1+\ldots+\xi_{n-1})\wedge\xi_n].$$



This area reflects the associative, but noncommutative properties of the operator product.

Projections of phase space polygons onto conjugate planes may have complex self-intersections:



The Weyl symbol of this product, $A_n \dots A_1(\mathrm{x})$,
the Fourier transform of the chord symbol,
is neatly written in terms of the multivariable function,

$$'A_n \dots A_1'(\mathrm{x}_n,\dots,\mathrm{x}_1) =$$

$$\int \frac{d\xi_n \dots d\xi_1}{(2\pi\hbar)^{nN}} \exp\left[\frac{-i}{\hbar} D_{n+1}(\xi_1,\dots,\xi_n)\right] \prod_{j=n}^{n} \widetilde{A}_j(\xi_j) \exp\left[-\frac{i}{\hbar} x_j \wedge \xi_j\right],$$

such that the Weyl representation of the product is just

$$'A_n \dots A_1'(\mathrm{x},\dots,\mathrm{x}) = A_n \dots A_1(\mathrm{x}).$$

Except for the polygonal factor, $'A_n \ldots A_1'(\mathrm{x}_n,\ldots,\mathrm{x}_1)$ would be just a product of Weyl symbols, $A_n(\mathrm{x}_n)\ldots A_1(\mathrm{x}_1)$. Thus, the full multiple Fourier transform is simply expressed as

$$'A_n \ldots A_1'(\mathrm{x}_n,\ldots,\mathrm{x}_1) = \exp\left[-i\hbar\, D_{n+1}\left(\frac{\partial}{\partial \mathrm{x}_1},\ldots,\frac{\partial}{\partial \mathrm{x}_n}\right)\right] A_n(\mathrm{x}_n)\ldots A_1(\mathrm{x}_n).$$

We have a multiple ***Groenewold-Moyal-star product.***

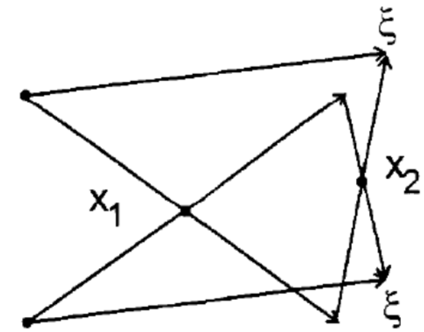
For a single pair of operators, we regain

$$A_2 A_1(\mathrm{x}) = \exp\left[-i\frac{\hbar}{2}\frac{\partial}{\partial \mathrm{x}_1}\wedge\frac{\partial}{\partial \mathrm{x}_2}\right] A_1(\mathrm{x}_1)|_{\mathrm{x}_1=\mathrm{x}}\, A_2(\mathrm{x}_2)|_{\mathrm{x}_2=\mathrm{x}}$$

What about direct use of the Weyl representation?
The simplest case is for an even number of operators:

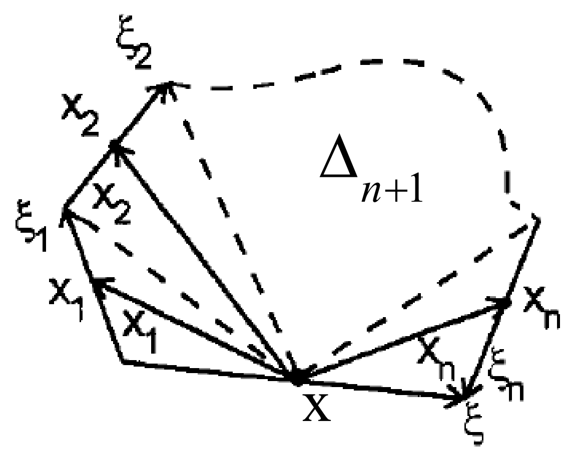
$$A_n \ldots A_1(\mathrm{x}) = \int \frac{d\mathrm{x}_n \ldots d\mathrm{x}_1}{(\pi\hbar)^{nN}} A_n(\mathrm{x}_n) \ldots A_1(\mathrm{x}_1) \,\mathrm{tr}\, \hat{R}_{\mathrm{x}} \hat{R}_{\mathrm{x}_n} \ldots \hat{R}_{\mathrm{x}_1}.$$

The properties of the quantum affine group
(*reflection x reflection = translation*)
(*reflection x translation = reflection*)
then lead to:



$$A_n \ldots A_1(\mathrm{x}) = \int \frac{d\mathrm{x}_n \ldots d\mathrm{x}_1}{(\pi\hbar)^{nN}} A_n(\mathrm{x}_n) \ldots A_1(\mathrm{x}_1) \exp\left[\frac{i}{\hbar}\Delta_{n+1}(\mathrm{x},\mathrm{x}_1,\ldots,\mathrm{x}_n)\right].$$

Again we have a polygon determining the phase, but $\Delta_{n+1}(\mathrm{x},\mathrm{x}_1,\ldots,\mathrm{x}_n)$ *is now specified by the centres of its sides.*



2. Path integral for the Weyl propagator: *semiclassical limit*

The ***Weyl Hamiltonian***, $H(\mathbf{x})$, is close
to the classical Hamiltonian, within order of $\hbar$.
In the limit of small times, the ***Weyl propagator***,
i.e., the Weyl symbol for the evolution operator, $\hat{U}_t$, is

$$U_t(\mathrm{x}) \xrightarrow[t\to 0]{} \exp\left[-i\frac{t}{\hbar}H(\mathrm{x})\right].$$

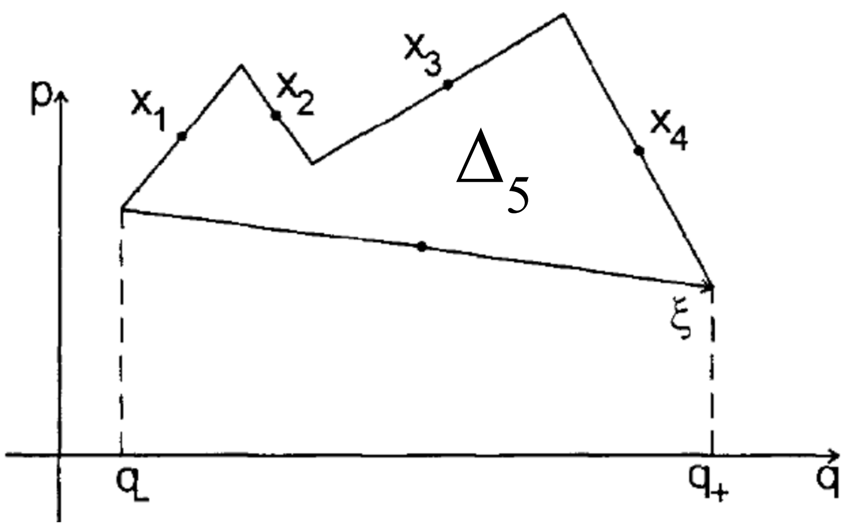
Then the path integral for finite times
is merely the product formula, itself:

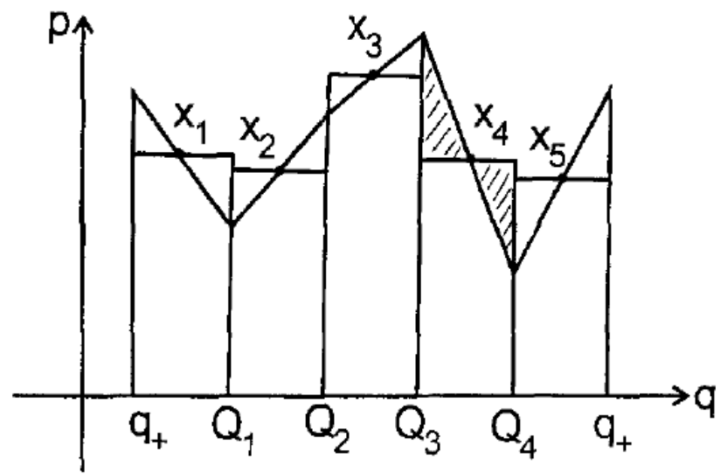
$$U_t(\mathrm{x}) = \lim_{n\to\infty} \int \frac{d\mathrm{x}_n \ldots d\mathrm{x}_1}{(\pi\hbar)^{nN}} \exp\left\{\frac{i}{\hbar}\left[\Delta_{n+1}(\mathrm{x},\mathrm{x}_1,\ldots,\mathrm{x}_n) - \frac{t}{n}\sum_{n'=1}^{n} H(x_{n'})\right]\right\}.$$

If the Hamiltonian separates into kinetic and potential energies,
this is the Weyl transform of the ***Feynman path integral***:

$$\langle q_+ | \hat{U}_t | q_- \rangle = \int \frac{dp}{(2\pi\hbar)^N} U_t(p, \frac{q_+ + q_-}{2}) \exp\left[-\frac{i}{\hbar} p \bullet (q_+ - q_-) \right].$$

The phase added in the transform fills in
the area between the polygon and the q-axis.
The full area can then be covered by thin strips.



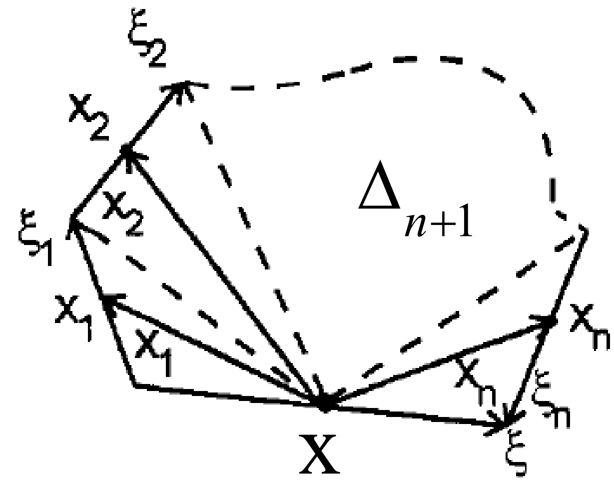


Stationary phase evaluation, for each centre x_j, demands that:

$$\mathbf{J}\frac{\partial \Delta_{n+1}}{\partial \mathrm{x}_j} = \xi_j = \frac{t}{n}\,\mathbf{J}\frac{\partial H}{\partial \mathrm{x}_j} = \frac{t}{n}\dot{\mathrm{x}}_j\,.$$

In short, the trajectory at each centre must be tangent to the respective side of the polygon.

In the limit, $n \to \infty$, *the stationary polygon defines a single classical trajectory, with its endpoints centred at* x.



The **semiclassical Weyl propagator** is then

$$U(\mathbf{x}) = \frac{2^N}{|\det(\mathbf{I}+\mathbf{M})|^{1/2}} \exp\left[\frac{\mathrm{i}}{\hbar}\left(S(\mathbf{x}) + \frac{\hbar\pi\sigma}{2}\right)\right].$$

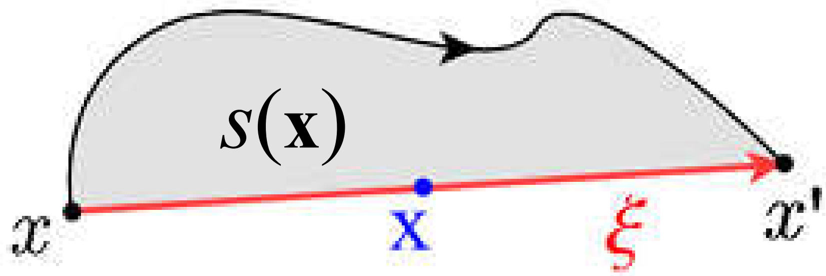
if there is a single trajectory with centre **x**

Berry

The **centre action** or **centre generating function**, $S(\mathbf{x})$, specifies a *finite evolution* through *'Hamilton's equations'*:

$$\boldsymbol{\xi} = -\mathbf{J}\frac{\partial S}{\partial \mathbf{x}}, \quad x' = \mathbf{x} + \frac{\boldsymbol{\xi}}{2}, \quad x = \mathbf{x} - \frac{\boldsymbol{\xi}}{2}.$$

The full **centre action** is $S(\mathbf{x}) = s(\mathbf{x}) - Et$.



*Usual generating functions specify a trajectory by a pair of positions, (**q, q'**) while momenta (**p, p'**) are free. Here, we have a fixed centre with free chord.*

The **monodromy matrix**, **M**, determines the linearized transformation, $x \mapsto x' = \mathbf{M}x$ between the tips of the classical trajectory.

3. Compound unitary operators

Multiple evolving correlations among observables:

$$\mathbf{C} = \langle \widehat{A}_\nu(t_\nu) \ldots \widehat{A}_2(t_2)\widehat{A}_1(t_1)\rangle = \mathrm{tr}\ \widehat{A}_\nu(t_\nu)\ \ldots\ \widehat{A}_2(t_2)\widehat{A}_1(t_1)\ \widehat{\rho}$$

where each of the operators $\widehat{A}_j(t_j)$
undergoes a Heisenberg evolution:

$$\widehat{A}_j(t) = \widehat{V}_j(t_j)^\dagger\ \widehat{A}_j\ \ \widehat{V}_j(t_j).$$

Define the intermediate steps:

$$\widehat{U}_{j+1} \equiv \widehat{V}_{j+1}(t_{j+1})\widehat{V}_j(t_j)^\dagger \quad (\text{with } \widehat{U}_1 \equiv \widehat{V}_1 \text{ and } \widehat{U}_{\nu+1} \equiv \widehat{V}_\nu(t_\nu)^\dagger)$$

then

$$\mathbf{C} = \mathrm{tr}\ \widehat{U}_{\nu+1}\widehat{A}_\nu\ \widehat{U}_\nu\ \ldots\ \widehat{A}_2\ \widehat{U}_2\ \widehat{A}_1\ \widehat{U}_1\ \widehat{\rho},$$

including Loschmidt echo, or fidelity.

Thus, the evolving correlation becomes

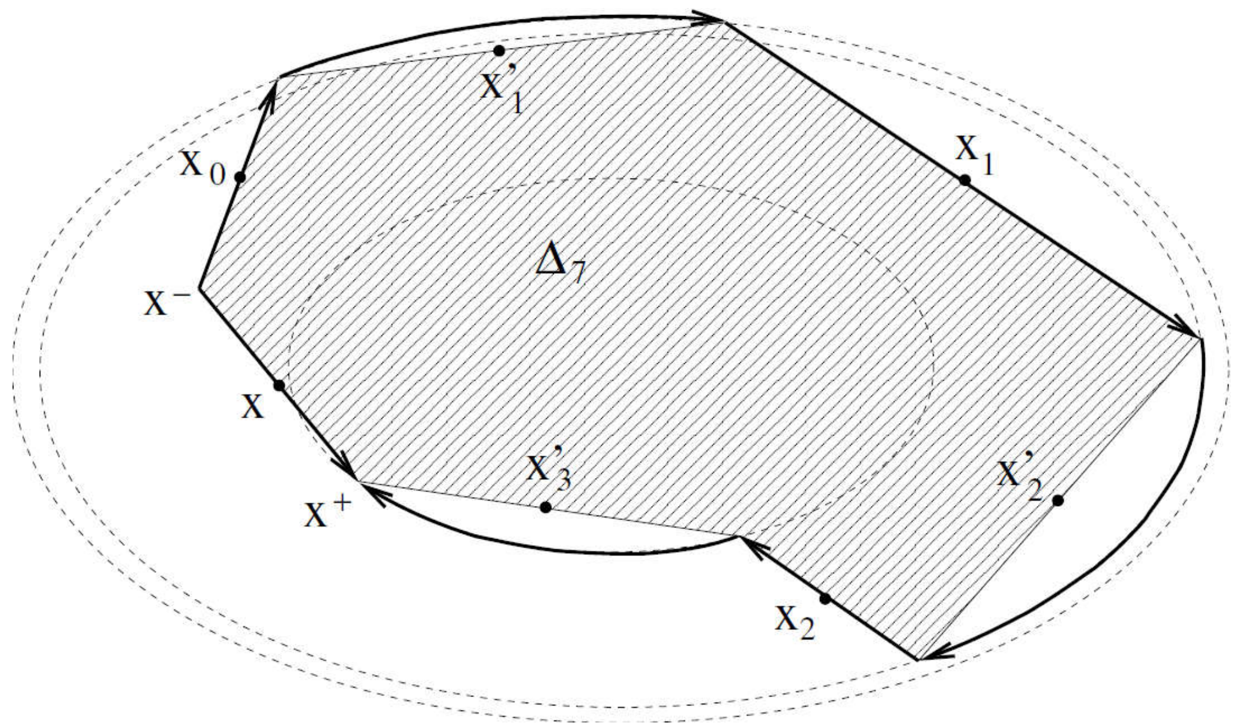
$$\mathbf{C} = \frac{2^N}{(\pi\hbar)^{\nu N}} \int d\mathbf{x}_\nu ... d\mathbf{x}_2 d\mathbf{x}_1 d\mathbf{x}_0 \; A_\nu(\mathbf{x}_\nu) ... A_2(\mathbf{x}_2) \; A_1(\mathbf{x}_1) \, W(\mathbf{x}_0)$$
$$\mathrm{tr} \, \widehat{\mathbf{U}}\{\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_\nu\},$$

where the kernel for the evolution for the initial correlation
is defined as

$$\widehat{\mathbf{U}}\{\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_\nu\} \equiv \widehat{U}_{\nu+1} \; \hat{R}_{\mathbf{x}_\nu} \; \widehat{U}_\nu ... \; \hat{R}_{\mathbf{x}_1} \widehat{U}_1 \; \hat{R}_{\mathbf{x}_0}.$$

But the reflection operators are also unitary, so that this sequence
can be considered as a single **compound unitary operator**.
It defines a quantum evolution corresponding to
a classical **compound canonical transformation**.

Assume that the compound Weyl propagator, $\mathbf{U}(\mathrm{x})$, shares the standard semiclassical form as each individualpropagator, $U_\nu(\mathrm{x}_\nu')$.



That is, assume that the compound classical action is

$$\mathbf{S}(\mathbf{x}) = \Delta_{2\nu+3} + S_1(\mathbf{x}'_1) + \ldots + S_{\nu+1}(\mathbf{x}'_{\nu+1})$$

Likewise, the amplitude of the compound propagator
is determined by the monodromy matrix of the full motion:
The product of the linearised transformation for each segment:

$$\mathbf{M} = [-\mathbf{I}] \cdot \mathbf{M}_1 \cdot [-\mathbf{I}] \cdot \mathbf{M}_2 \cdot \ldots [-\mathbf{I}] \cdot \mathbf{M}_{\nu+1}$$

reflections *evolutions*

The monodromy matrices for the reflections are independent of the position of their reflection centres, but **M** and $S(\mathrm{x})$ depend on all the centres $\{\mathrm{x}_0, \mathrm{x}_1, \mathrm{x}_2, ..., \mathrm{x}_\nu\}$, that parametrize a *family of canonical transformations*.

Now one requires tr $\hat{\mathbf{U}}$, but the trace of any operator equals the phase space integral of its Weyl representation:

$$\mathrm{tr}\ \widehat{U} = \int \frac{d\mathbf{x}}{(2\pi\hbar)^N}\ U(\mathbf{x})$$

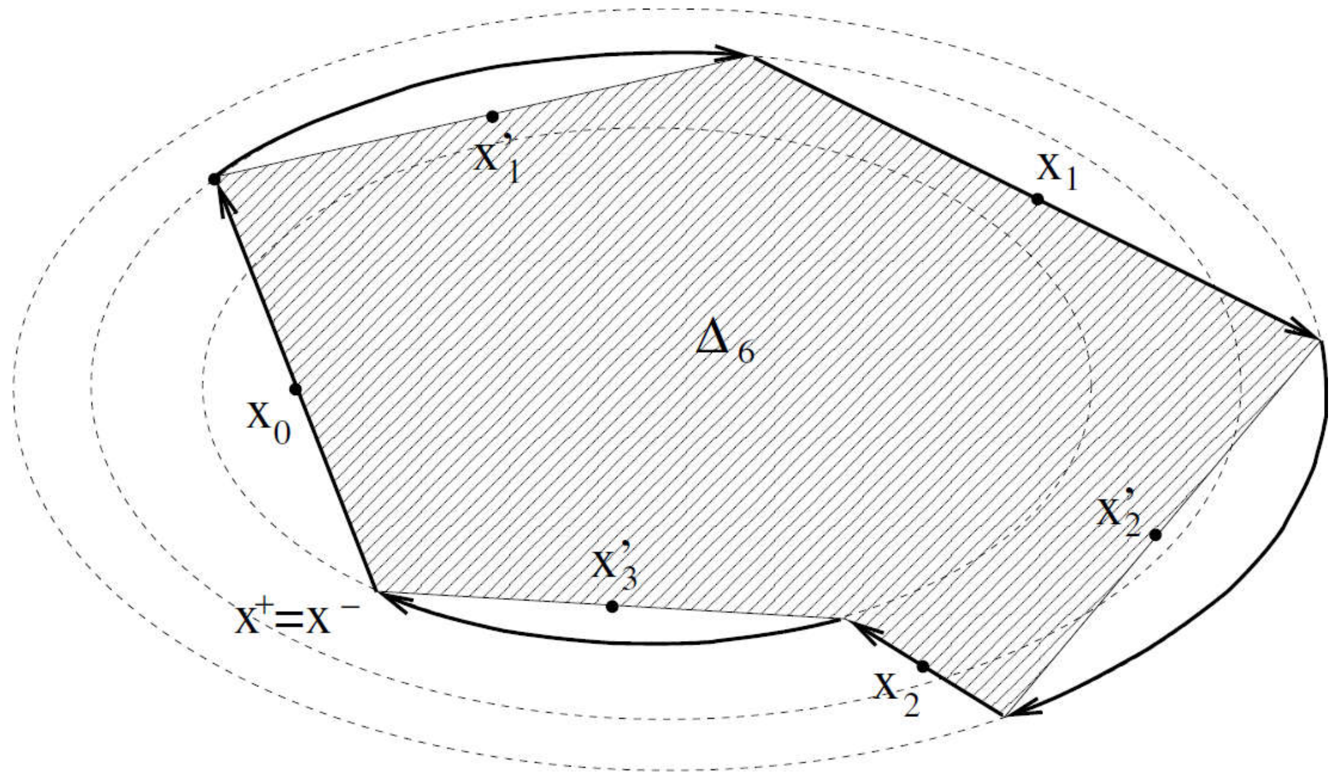
The only explicit dependence of $\mathbf{U}$(x) on x lies in $\Delta_{2n+3} = \mathbf{x} \wedge \boldsymbol{\xi} + C$
Since the chord centred on $\mathbf{x}$ depends only on the other centres,

$$\frac{\boldsymbol{\xi}}{2} = (\mathbf{x}'_1 - \mathbf{x}_0) + (\mathbf{x}'_2 - \mathbf{x}_1) + ... + (\mathbf{x}'_{\nu+1} - \mathbf{x}_\nu)$$

then

$$\int \frac{d\mathbf{x}}{(2\pi\hbar)^N}\ \exp\left[\frac{i\Delta_{2\nu+3}(\mathbf{x}, \mathbf{x}_j, \mathbf{x}'_j)}{\hbar}\right] = \exp\left[\frac{i\Delta_{2\nu+2}(\mathbf{x}_j, \mathbf{x}'_j)}{\hbar}\right] \delta(\boldsymbol{\xi})$$

But if the chord centred on x is zero, the selected trajectory is periodic!



Then stationary phase evaluation:

$$\mathrm{tr}\,\widehat{\mathbf{U}}_p \approx \frac{2^N}{|\det(\mathbf{I}-\mathbf{M})|^{1/2}} \exp\left[\frac{i}{\hbar}(\mathbf{S}(\mathbf{x}) + \frac{\hbar\pi\sigma'}{4})\right]$$

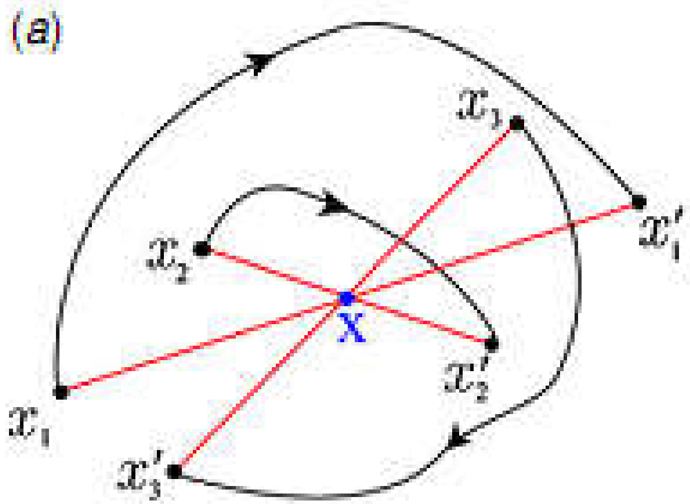
4. Initial value representation

The appropriate trajectories for a semiclassical propagator are determined by boundary conditions. If the finite evoution is specified by Hamilton’s *differential* equations, there is a practical ***root search problem*** to find the trajectory.

Also, in the case of the trace, one must search for the periodic trajectories.

A further problem concerns ***caustics:***

There may be several trajectories with the same centre:



A pair of chords coalesces for a centre**,** **x**, on a ***centre caustic***.

The caustic singularities of the Weyl propagator are loci of centres, at which an eigenvalue of **M**, $\lambda = -1$.

In the case of the trace of the propagator, the caustics arise at ***periodic orbit bifurcations***: They occur along codimension-1 surfaces in the parameter space $\{\mathrm{x}_0, \mathrm{x}_1, \mathrm{x}_2, \ldots, \mathrm{x}_\nu\}$

Let us then reinterpret tr $\hat{\mathbf{U}}$ as the Weyl representation of a *reduced compound unitary operator*:

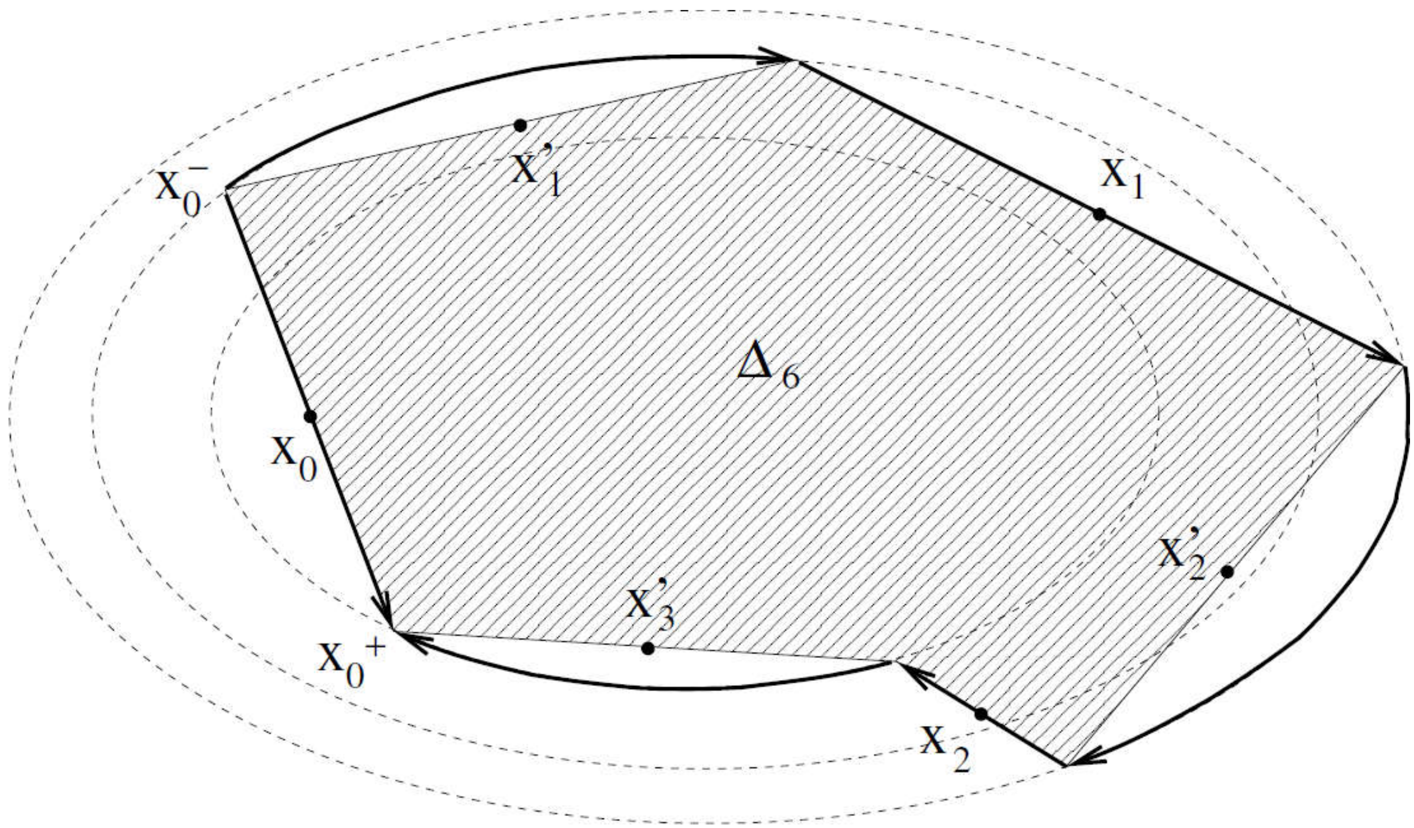
$$\mathrm{tr}\ \widehat{\mathbf{U}}\{\mathbf{x}_0, \mathbf{x}_1, ..., \mathbf{x}_\nu\} = \mathrm{tr}\ \widehat{U}_{\nu+1}\ \hat{R}_{\mathbf{x}_\nu}\ \widehat{U}_\nu ...\ \hat{R}_{\mathbf{x}_1} \widehat{U}_1\ \hat{R}_{\mathbf{x}_0} = \mathbf{U}'(\mathbf{x}_0)$$

that is,

$$\widehat{\mathbf{U}'} \equiv \widehat{U}_{\nu+1}\ \hat{R}_{\mathbf{x}_\nu}\ \widehat{U}_\nu ...\ \hat{R}_{\mathbf{x}_1} \widehat{U}_1.$$

This has one less reflection than $\hat{\mathbf{U}}$**,** but it has an analogous semiclassical approximation:

The same figure as before is now interpreted as an open polygonal line, going from x_0^- to x_0^+.



Each branch of the generating function $S(x_0)$ is constructed from a compound trajectory that satisfies $x_0^- + x_0^+ = 2\,x_0$.
But there is still a root search and caustics…

The *initial value representation* (IVR) now results from the change of variable in the integral for the correlation

$$\mathbf{C} = \frac{2^N}{(\pi\hbar)^{\nu N}} \int d\mathbf{x}_\nu ... d\mathbf{x}_2 d\mathbf{x}_1 d\mathbf{x}_0 \; A_\nu(\mathbf{x}_\nu)...A_2(\mathbf{x}_2)\, A_1(\mathbf{x}_1)\, W(\mathbf{x}_0)$$

$$\mathrm{tr}\, \widehat{\mathbf{U}}\{\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_\nu\},$$

from the trajectory midpoint, $\mathbf{x}_0$ to the initial point, $\boldsymbol{x}_0{}^-$.
Thus, one changes the integration variable to the **initial value** of the classical trajectory: The Jacobian is

$$\det\left(\frac{\partial \mathrm{x}_0}{\partial \mathrm{x}_0^-}\right) = \det\left(\frac{\mathbf{I}+\mathbf{M}}{2}\right)$$

Thus, the semiclassical approximation for the evolving correlation becomes:

$$\mathbf{C} = \frac{2^N}{(\pi\hbar)^{\nu N}} \int d\mathbf{x}_\nu \ldots d\mathbf{x}_1 d\boldsymbol{x}_{\bar{0}} \; A_\nu(\mathbf{x}_\nu) \ldots A_1(\mathbf{x}_1)\, W(\mathbf{x}_0(\boldsymbol{x}_{\bar{0}}))|\mathbf{I}+\mathbf{M}'|^{1/2} \exp\left[\frac{i}{\hbar}(\mathbf{S}'(\mathbf{x}_0(\boldsymbol{x}_{\bar{0}})) + \hbar\pi\sigma)\right]$$

where now all classical variables are determined by the initial value of the compound trajectory: $\mathrm{x}_{\bar{0}}$.

No more root search and no more caustics!

5. An example: IVR for the quantum fidelity

The *Loschmidt echo* for different forward and back evolutions,

$$L(t) = \left\langle \psi \middle| \left\langle \exp\left(\frac{i}{\hbar}\hat{H}_+ t\right) \exp\left(-\frac{i}{\hbar}\hat{H}_- t\right) \middle| \psi \right\rangle\right.$$

can be expressed in terms of an *echo operator,*

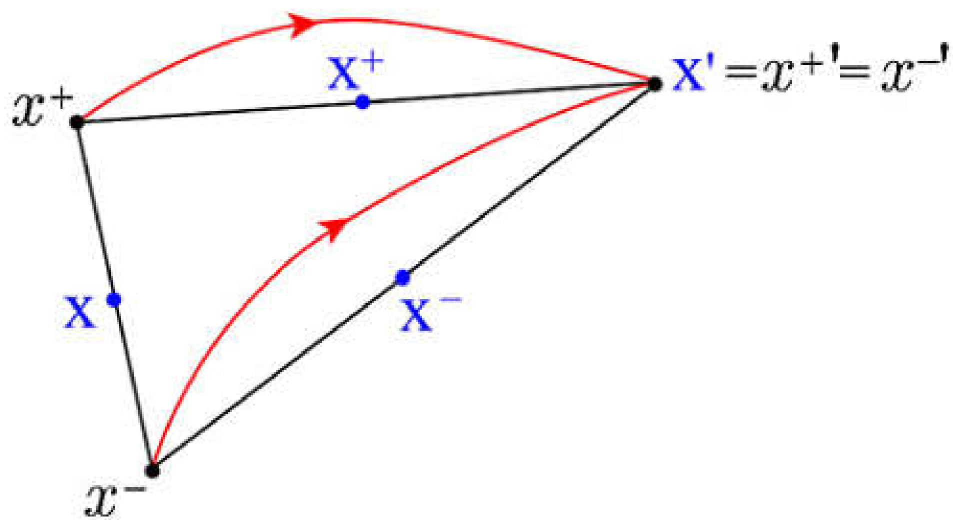
$$\widehat{I}_L(t) = \widehat{U}_+(t)^\dagger\, \widehat{I}\, \widehat{U}_-(t) = \exp\left(\frac{\mathrm{i}}{\hbar}\widehat{H}_+ t\right) \widehat{I}\, \exp\left(-\frac{\mathrm{i}}{\hbar}\widehat{H}_- t\right),$$

a simple compound operator, with $\hat{I} = \hat{T}_0$, *instead of* $\hat{R}_{\mathrm{x}}$ *:*

$$L(t) = \mathrm{tr}\left[\widehat{\rho}\, \widehat{I}_L(t)\right] = \int \frac{\mathrm{d}\mathbf{x}}{(\pi\hbar)^N}\; W(\mathbf{x}) I_L(\mathbf{x}, t).$$

Thus, we obtain the IVR:

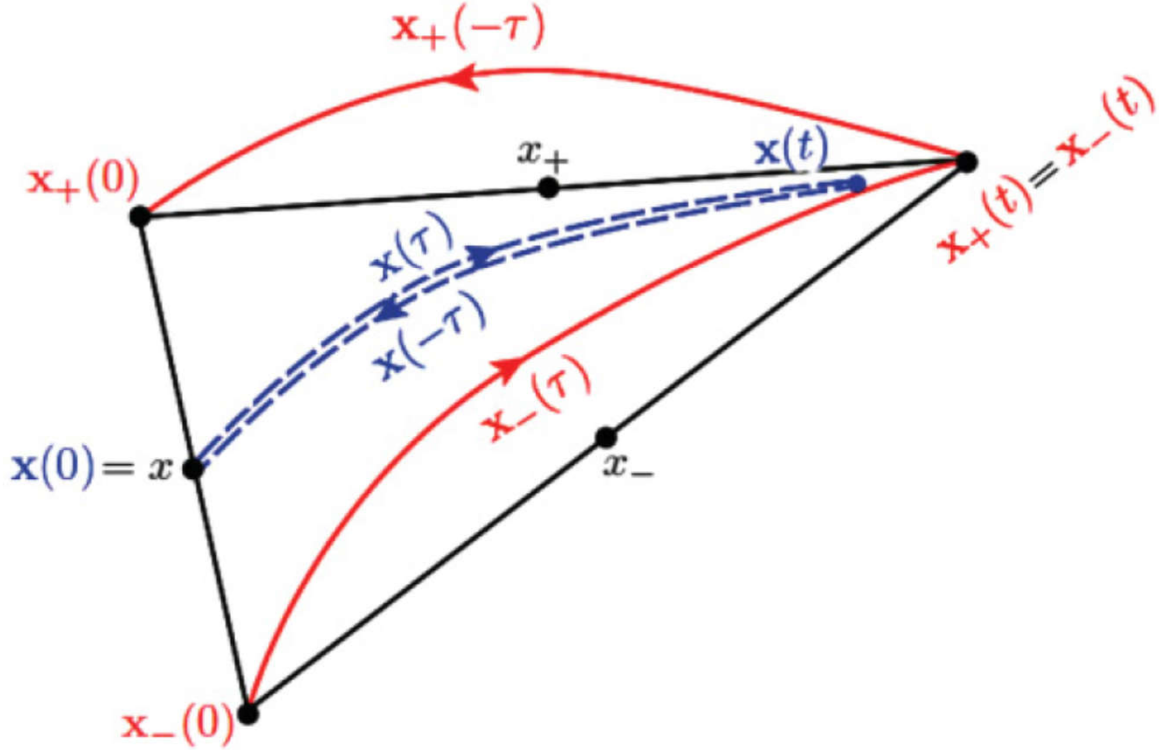
$$L(t) = \int \frac{\mathrm{d}\boldsymbol{x}^-}{(2\pi\hbar)^N} \sqrt{|\det(\mathbf{I} + [\mathbf{M}_+(\mathbf{x}^+)]^{-1}\, \mathbf{M}_-(\mathbf{x}^-))|}$$
$$\times \exp\left\{\frac{\mathrm{i}}{\hbar}\left[S_0\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) + \frac{\hbar\sigma\pi}{2}\right]\right\} W\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right).$$



This is exact for a pair of harmonic oscilators.

Vaniceck's *dephasing representation* results
by *approximating the action within classical perturbation theory as the time integral of* $\delta H = H^{+}(x) - H^{-}(x)$ *along a single trajectory:*

$$L_{\mathrm{DR}}(t) = \int dx_0 W(x_0) \exp\left(-\frac{i}{\hbar}\int_0^t \delta H(\mathbf{x}(\tau;x_0))d\tau\right)$$



5. Discussion:

The exchange of focus from the individual semiclassical propagator to complete evolving correlations pays off!
Some care needs still to be taken:

i. General rules for phase evaluation through caustics:
These become zeroes of the integrand, leading to sign changes:

i. Numerical computations for nonlinear evolutions
(Comparison with Hermann-Kluk computations).

iii. Adaptation to nonunitary *(Markovian)* evolution.

iv. Semiclassical evaluation for reduced density operators.

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