Phase space path integrals and their semiclassical approximations

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[1] N. Kumano-go and D. Fujiwara, Phase space Feynman path integrals via piecewise bicharacteristic paths and their semiclassical approximations. Bulletin des Sciences Mathematique, In press, Available online 2007.

1. Introduction

Let $u(T)$ be the solution for the Schrödinger equation

$$(i\hbar\partial_T - H(T, x, \frac{\hbar}{i}\partial_x))u(T) = 0\,, \quad u(0) = v\,.$$

In the theory of Fourier integral operators, we write $u(T)$ as

$$u(T) = \left(\frac{1}{2\pi\hbar}\right)^d \int_{\mathrm{R}^d}\int_{\mathrm{R}^d} K(T, x, \xi_0, x_0)v(x_0)dx_0 d\xi_0\,.$$

Using the phase space path integral, we formally write $K(T, x, \xi_0, x_0)$ as

$$K(T, x, \xi_0, x_0) = \int e^{\frac{i}{\hbar}\phi[q,p]}\mathcal{D}[q, p]\,.$$

Here $(q, p) : [0, T] \to \mathrm{R}^{2d}$ is the path with $q(0) = x_0$, $q(T) = x$ and $p(0) = \xi_0$,

$$\phi[q, p] = \int_{[0,T)} p(t)\cdot dq(t) - \int_{[0,T)} H(t, q(t), p(t))dt\,,$$

and the phase space path integral $\int \sim \mathcal{D}[q, p]$ is a sum over all paths (q, p).

Our results Using piecewise bicharacteristic paths, we prove the existence of the phase space path integrals

$$\int e^{\frac{i}{\hbar}\phi[q,p]} F[q,p] \mathcal{D}[q,p] \,,$$

with general functional $F[q,p]$ as integrand. More precisely, we give a fairly general class $\mathcal{F}$ such that for any $F[q,p] \in \mathcal{F}$, the time slicing approximation converges uniformly on compact subsets of the endpoints (x, ξ_0, x_0).

Other mathematical definitions of phase space path integral

- Daubechies-Klauder The definition via analytic continuation from the phase space Wiener measure.
- Albeverio-Guatteri-Mazzucchi

The definition via Fresnel integral transform

- Smolyanov-Tokarev-Truman The definition via Chernoff formula • • •

2. Existence of phase space path integrals

Assumption $H(t,x,\xi): \mathrm{R}\times\mathrm{R}^d\times\mathrm{R}^d\to\mathrm{R}$, $\partial_x^\alpha\partial_\xi^\beta H(t,x,\xi)$:continuous

$$|\partial_x^\alpha\partial_\xi^\beta H(t,x,\xi)|\le C_{\alpha,\beta}(1+|x|+|\xi|)^{\max(2-|\alpha+\beta|,0)}\,.$$

Examples

$$H(t,x,\frac{\hbar}{i}\partial_x)=\sum_{j,k=1}^{d}(a_{j,k}(t)\frac{\hbar}{i}\partial_{x_j}\frac{\hbar}{i}\partial_{x_k}+b_{j,k}(t)x_j\frac{\hbar}{i}\partial_{x_k}+c_{j,k}(t)x_jx_k)$$
$$+\sum_{j=1}^{d}(a_j(t)\frac{\hbar}{i}\partial_{x_j}+b_j(t)x_j)+c(t,x)\,.$$

Here $a_{j,k}(t)$, $b_{j,k}(t)$, $c_{j,k}(t)$, $a_j(t)$, $b_j(t)$ and $\partial_x^\alpha c(t,x)$ are real-valued continuous bounded functions.

We can produce many $F[q,p] \in \mathcal{F}$

We will define the class $\mathcal{F}$ in the last section. Because, even if we do not state the definition of $\mathcal{F}$ here, we can produce many functionals $F[q,p] \in \mathcal{F}$.

Examples of $F[q,p] \in \mathcal{F}$

(1) The functionals of (t,q) independent of p,

$$F[q] = B(t, q(t)) \in \mathcal{F}\,, \quad F[q,p] \equiv 1 \in \mathcal{F}\,.$$

(2) The Riemann integrals $F[q,p] = \displaystyle\int_{T'}^{T''} B(t, q(t), p(t))dt \in \mathcal{F}$.

(3) If $B(t,x,\xi)$ is bounded, then $F[q,p] = e^{\int_{T'}^{T''} B(t,q(t),p(t))dt} \in \mathcal{F}$.

Theorem 1 $F[q,p], G[q,p] \in \mathcal{F} \Longrightarrow F[q,p] + G[q,p], F[q,p]G[q,p] \in \mathcal{F}$.

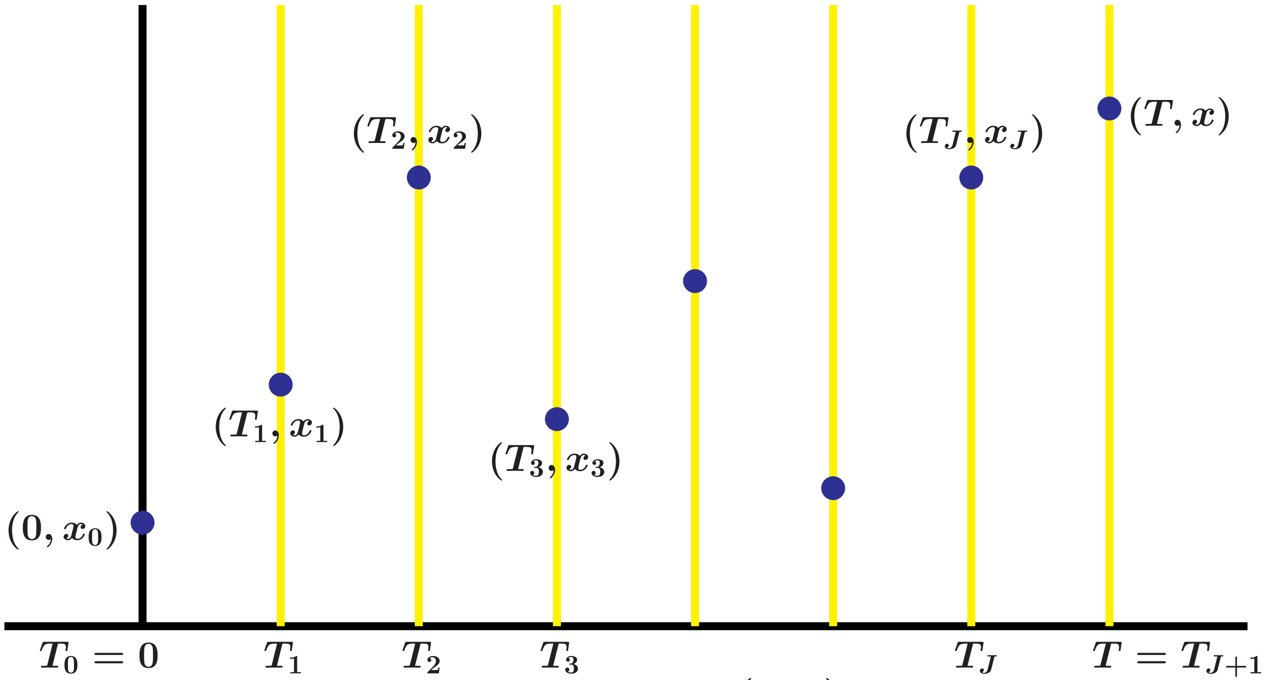
The time slicing approximation

Let $\Delta_{T,0} = (T_{J+1}, T_J, \ldots, T_1, T_0)$ be any division of the interval $[0, T]$.

$$\Delta_{T,0} : T = T_{J+1} > T_J > \cdots > T_1 > T_0 = 0\,.$$

Set $t_j = T_j - T_{j-1}$ for $j = 1, 2, \ldots, J+1$. Let $|\Delta_{T,0}| = \max_{1 \le j \le J+1} t_j$.

Set $x_{J+1} = x$. Let $x_j \in \mathrm{R}^d$ and $\xi_j \in \mathrm{R}^d$ for $j = 1, 2, \ldots, J+1$.



The time slicing on (t, q)-space

The bicharacteristic paths

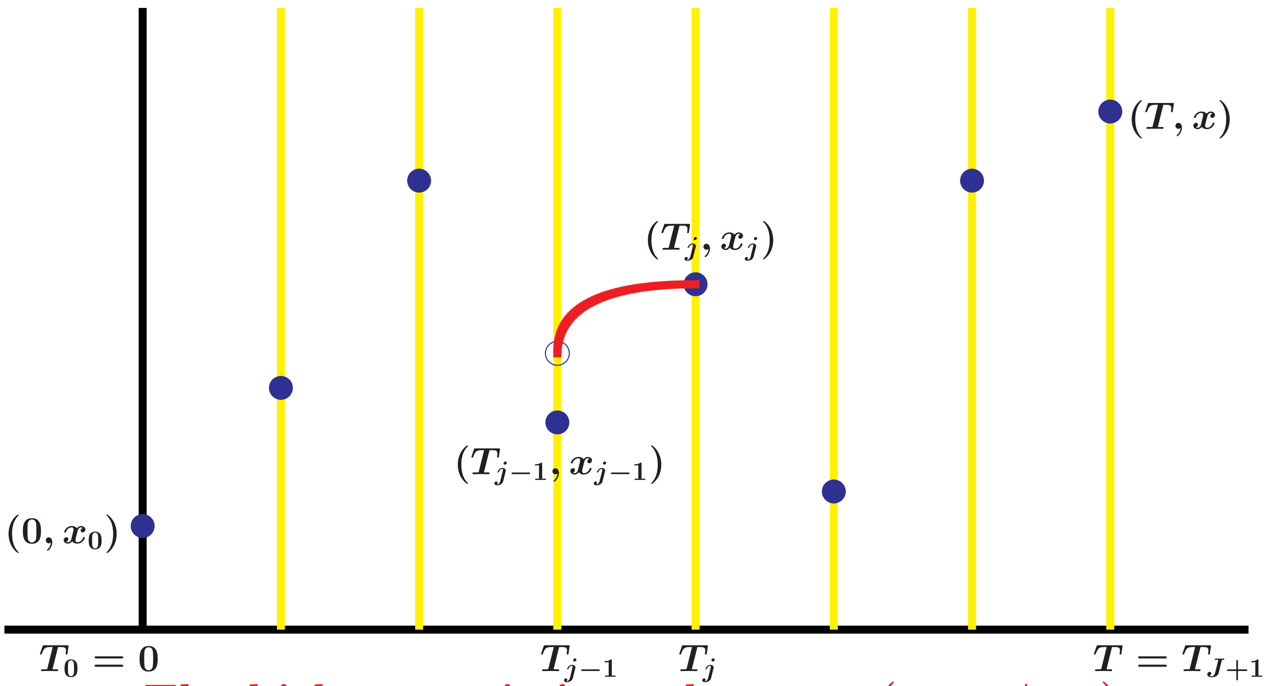
Assume $\kappa_2 d(T_j - T_{j-1}) < 1/2$.

Let $\bar{q}_{T_j,T_{j-1}}(t,x_j,\xi_{j-1})$, $\bar{p}_{T_j,T_{j-1}}(t,x_j,\xi_{j-1})$ satisfy the canonical equation

$$\partial_t \bar{q}_{T_j,T_{j-1}}(t) = (\partial_\xi H)(t, \bar{q}_{T_j,T_{j-1}}, \bar{p}_{T_j,T_{j-1}}),$$

$$\partial_t \bar{p}_{T_j,T_{j-1}}(t) = -(\partial_x H)(t, \bar{q}_{T_j,T_{j-1}}, \bar{p}_{T_j,T_{j-1}}), \quad T_{j-1} \le t \le T_j,$$

$$\bar{q}_{T_j,T_{j-1}}(T_j) = x_j, \quad \bar{p}_{T_j,T_{j-1}}(T_{j-1}) = \xi_{j-1}\,.$$



The bicharacteristic path $\bar{q}_{T_j,T_{j-1}}(t,x_j,\xi_{j-1})$

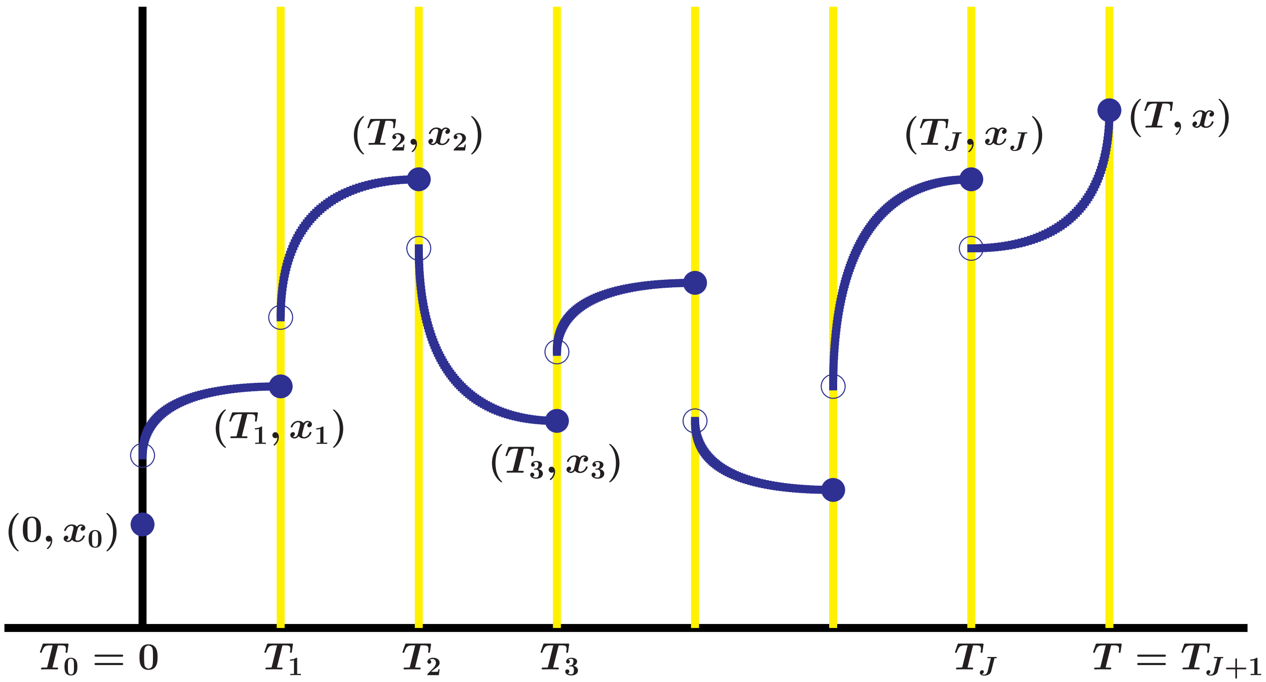
The piecewise bicharacteristic paths

We define

$q_{\Delta_{T,0}} = q_{\Delta_{T,0}}(t, x_{J+1}, \xi_J, \dots, x_1, \xi_0, x_0)$, $p_{\Delta_{T,0}} = p_{\Delta_{T,0}}(t, x_{J+1}, \xi_J, \dots, x_1, \xi_0)$ by

$$q_{\Delta_{T,0}}(t) = \bar{q}_{T_j, T_{j-1}}(t, x_j, \xi_{j-1}), \quad T_{j-1} < t \le T_j, \quad q_{\Delta_{T,0}}(0) = x_0$$

$$p_{\Delta_{T,0}}(t) = \bar{p}_{T_j, T_{j-1}}(t, x_j, \xi_{j-1}), \quad T_{j-1} \le t < T_j, \quad j = 1, 2, \dots, J, J+1.$$



The piecewise bicharacteristic path $q_{\Delta_{T,0}}$

Feynman path integrals exist

Theorem 2 Let T sufficinetly small. Then, for any $F[q,p] \in \mathcal{F}$,

$$(\star) \quad \int e^{\frac{i}{\hbar}\phi[q,p]} F[q,p] \mathcal{D}[q,p]$$

$$\equiv \lim_{|\Delta_{T,0}|\to 0} \left(\frac{1}{2\pi\hbar}\right)^{d/2} \int_{\mathrm{R}^{2dJ}} e^{\frac{i}{\hbar}\phi[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}]} F[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}] \prod_{j=1}^{J} d\xi_j dx_j$$

converges unifomly on compact sets of (x, ξ_0, x_0), i.e., well-defined.

Remark Even when $F[q,p] \equiv 1$, each integral of right hand side of $(\star)$

does not converge absolutely. (Oscillatory integral)

$$\int_{\mathrm{R}^{2d}} 1 d\xi_j dx_j = \infty$$

Furthermore, the number J of integrals (division points) tends to infinity.

$$\infty \times \infty \times \infty \times \infty \times \cdots\cdots\cdots, \quad J \to \infty.$$

Remark The functionals $\phi[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}]$, $F[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}]$ are functions, i.e.,

$$\phi[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}] = \phi_{\Delta_{T,0}}(x_{J+1}, \xi_J, x_J, \ldots, \xi_1, x_1, \xi_0, x_0),$$

$$F[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}] = F_{\Delta_{T,0}}(x_{J+1}, \xi_J, x_J, \ldots, \xi_1, x_1, \xi_0, x_0),$$

In order to treat the integrals one by one as an operator, the Trotter formula uses a sum of functions as an approximation, e.g.,

$$\sum_{j=1}^{J+1}(x_j - x_{j-1})\xi_{j-1} - (t_j - t_{j-1})\frac{\xi_{j-1}^2}{2} - (t_j - t_{j-1})V(x_{j-1}).$$

However the operator does not distinguish the configuration paths and the phase space paths.

In our approach, treating the multiple integral directly, we keep the phase space paths in the functionals $\phi[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}]$, $F[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}]$ of the multiple integral.

3. Interchange of the order with Riemann integrals

Theorem 3 $m \geq 0$, $0 \leq T' \leq T'' \leq T$, $B(t,x) : [0,T] \times \mathrm{R}^d \to \mathrm{C}$,

$\partial_x^\alpha B(t,x)$:continuous, $|\partial_x^\alpha B(t,x)| \leq C_\alpha (1+|x|)^m$, Let T sufficiently small.

Then

$$\int e^{\frac{i}{\hbar}\phi[q,p]} \left(\int_{T'}^{T''} B(t,q(t))dt \right) \mathcal{D}[q,p] = \int_{T'}^{T''} \left(\int e^{\frac{i}{\hbar}\phi[q,p]} B(t,q(t)) \mathcal{D}[q,p] \right) dt$$

Remark We can also interchange the order with an analytic limit.

Therefore, if $|\partial_x^\alpha B(t,x)| \leq C_\alpha$,

$$\begin{aligned} &\int e^{\frac{i}{\hbar}\phi[q,p] + \frac{i}{\hbar}\int_0^T B(\tau,q(\tau))d\tau} \mathcal{D}[q,p] \\ &= \sum_{n=1}^{\infty} \left(\frac{i}{\hbar}\right)^n \int_0^T d\tau_n \int_0^{\tau_n} d\tau_{n-1} \cdots \int_0^{\tau_2} d\tau_1 \\ &\times \int e^{\frac{i}{\hbar}\phi[q,p]} B(\tau_n, q(\tau_n)) B(\tau_{n-1}, q(\tau_{n-1})) \cdots B(\tau_1, q(\tau_1)) \mathcal{D}[q,p] \,. \end{aligned}$$

Proof of Theorem 3 For simplicity, set $0 = T' < T'' = T$.

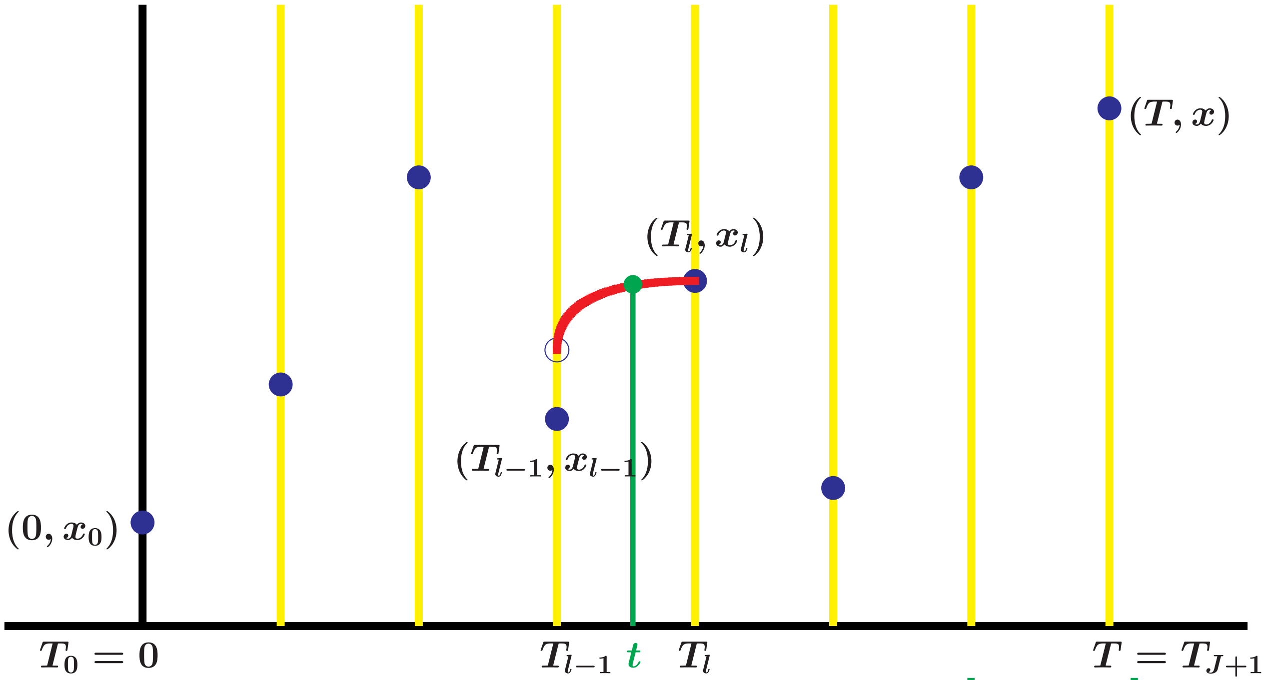
By Theorem 2, we have

$$\int e^{\frac{i}{\hbar}\phi[q,p]} \left(\int_0^T B(t, q(t))dt\right) \mathcal{D}[q,p]$$
$$= \lim_{|\Delta_{T,0}|\to 0} \left(\frac{1}{2\pi\hbar}\right)^{dJ} \int_{\mathrm{R}^{2dJ}} e^{\frac{i}{\hbar}\phi[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}]} \int_0^T B(t, q_{\Delta_{T,0}}(t))dt \prod_{j=1}^{J} d\xi_j dx_j \,.$$

We devide the interval $[0, T]$ into the subintervals $[T_{l-1}, T_l]$, $l = 1, 2, \ldots, J+1$.

$$= \lim_{|\Delta_{T,0}|\to 0} \sum_{l=1}^{J+1} \left(\frac{1}{2\pi\hbar}\right)^{dJ} \int_{\mathrm{R}^{2dJ}} e^{\frac{i}{\hbar}\phi[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}]} \int_{T_{l-1}}^{T_l} B(t, \bar{q}_{T_l, T_{l-1}}(t))dt \prod_{j=1}^{J} d\xi_j dx_j \,.$$

Since we do not approximate $\bar{q}_{T_l,T_{l-1}}(t)$ by the endpoint x_l or x_{l-1}, $B(t, \bar{q}_{T_l,T_{l-1}}(t))$ is continuous on $[T_l, T_{l-1}]$, together with all its derivatives in x_l and ξ_{l-1}.



The particle moves continuously on $[T_{l-1}, T_l]$

Therefore, we can interchange the order of the Riemann integration on $[T_{l-1}, T_l]$ and the oscillatory integration on R^{2dJ}.

$$= \lim_{|\Delta_{T,0}|\to 0} \sum_{l=1}^{J+1} \int_{T_{l-1}}^{T_l} \left(\frac{1}{2\pi\hbar}\right)^{dJ} \int_{\mathrm{R}^{2dJ}} e^{\frac{i}{\hbar}\phi[q_{\Delta_{T,0}},p_{\Delta_{T,0}}]} B(t,\bar{q}_{T_l,T_{l-1}}(t)) \prod_{j=1}^{J} d\xi_j dx_j dt$$

$$= \lim_{|\Delta_{T,0}|\to 0} \int_0^T \left(\frac{1}{2\pi\hbar}\right)^{dJ} \int_{\mathrm{R}^{2dJ}} e^{\frac{i}{\hbar}\phi[q_{\Delta_{T,0}},p_{\Delta_{T,0}}]} B(t,q_{\Delta_{T,0}}(t)) \prod_{j=1}^{J} d\xi_j dx_j dt\,.$$

By Theorem 2, the convergence of the time slicing approximation is uniform with respect to t on $[0,T]$. Therefore, we can interchange the order of $\lim_{|\Delta_{T,0}|\to 0}$ and $\int_0^T \sim dt$.

$$= \int_0^T \lim_{|\Delta_{T,0}|\to 0} \left(\frac{1}{2\pi\hbar}\right)^{dJ} \int_{\mathrm{R}^{2dJ}} e^{\frac{i}{\hbar}\phi[q_{\Delta_{T,0}},p_{\Delta_{T,0}}]} B(t,q_{\Delta_{T,0}}(t)) \prod_{j=1}^{J} d\xi_j dx_j dt$$

$$= \int_0^T \left(\int e^{\frac{i}{\hbar}\phi[q,p]} B(t,q(t)) \mathcal{D}[q,p]\right) dt\,. \ \square$$

4. Semiclassical approximation $\hbar \to 0$

Let $4\kappa_2 dT < 1/2$. Then, for any $(x_{J+1}, \xi_0) \in \mathrm{R}^d \times \mathrm{R}^d$, there exists the stationary point $(x_J^*, \xi_J^*, \ldots, x_1^*, \xi_1^*)$ of the phase function $\phi_{\Delta_{T,0}}$, i.e.,

$$(\partial_{(x_{J,1}, \xi_{J,1})} \phi_{\Delta_{T,0}})(x_{J+1}, \xi_J^*, x_J^*, \ldots, \xi_1^*, x_1^*, \xi_0) = 0 \,.$$

We define $D_{\Delta_{T,0}}(x_{J+1}, \xi_0)$ by

$$D_{\Delta_{T,0}}(x_{J+1}, \xi_0) = (-1)^{dJ} \det(\partial^2_{(\xi_J, x_J, \ldots, \xi_1, x_1)} \phi_{\Delta_{T,0}})(x_{J+1}, x_J^*, \xi_J^*, \ldots, x_1^*, \xi_1^*, \xi_0) \,.$$

Lemma There exists a limit function $D(T, x, \xi_0)$ such that

$$|\partial_x^\alpha \partial_{\xi_0}^\beta (D_{\Delta_{T,0}}(x, \xi_0) - D(T, x, \xi_0))| \le C_{\alpha,\beta} |\Delta_{T,0}| T \,,$$

We use this limit function $D(T, x, \xi_0) = \lim_{|\Delta_{T,0}| \to 0} D_{\Delta_{T,0}}(x, \xi_0)$ as a Hamiltonian version of the Morette-Van Vleck determinant.

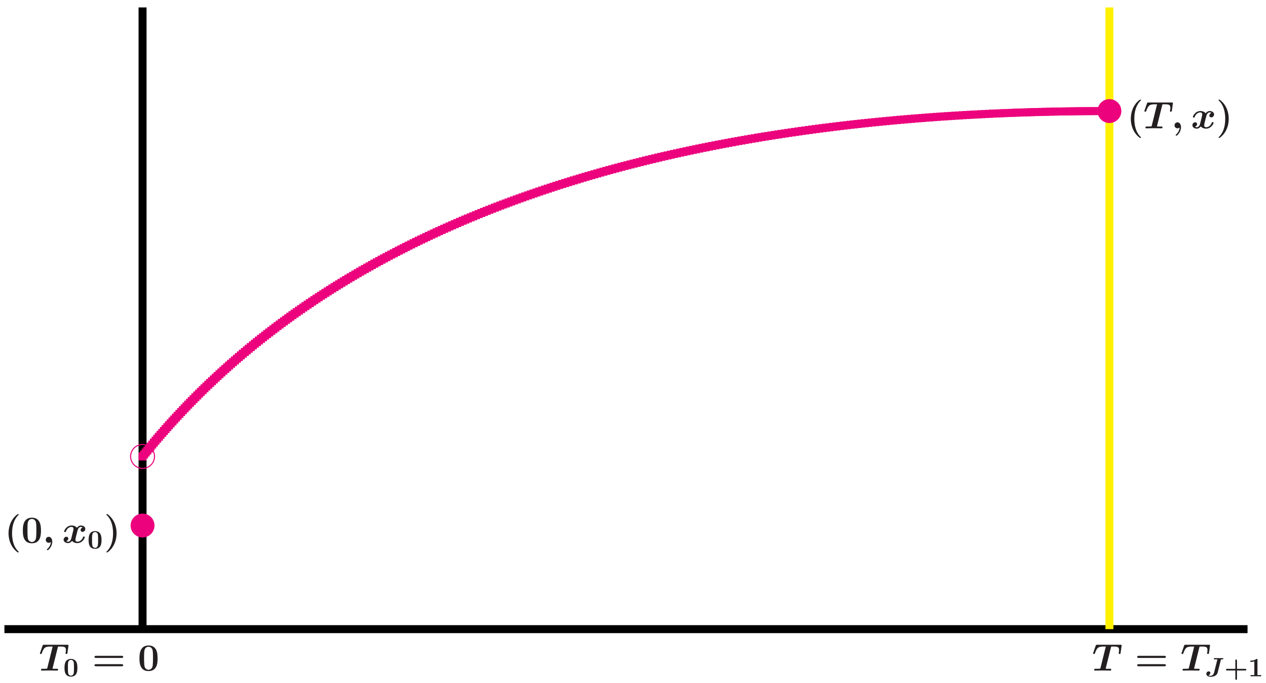
Theorem 4 (Semiclassical approximation $\hbar \to 0$)

Let T be sufficiently small. Then, for any $F[q,p] \in \mathcal{F}$,

$$\int e^{\frac{i}{\hbar}\phi[q,p]} F[q,p]\mathcal{D}[q,p] = e^{\frac{i}{\hbar}\phi[q_{T,0},p_{T,0}]}(D(T,x,\xi_0)^{-1/2} F[q_{T,0},p_{T,0}] + \hbar\Upsilon(\hbar,x,\xi_0,x_0)).$$

Here $q_{T,0} = q_{T,0}(t,x,\xi_0,x_0)$, $p_{T,0} = p_{T,0}(t,x,\xi_0)$ is the piecewise bicharacteristic path for the simplest division $0 < T$ and

$$|\partial_x^\alpha \partial_{\xi_0}^\beta \Upsilon(T,\hbar,x,\xi_0,x_0)| \le C_{\alpha,\beta}(1+|x|+|\xi_0|+|x_0|)^m .$$



The path $q_{T,0}$ for the simples division $0 < T$.

5. Proof of Theorem 1,2,4

In order to prove the convergence of the multiple integral

$$(\star) \quad \lim_{|\Delta_{T,0}|\to 0} \left(\frac{1}{2\pi\hbar}\right)^{d/2} \int_{\mathrm{R}^{2dJ}} e^{\frac{i}{\hbar}\phi[q_{\Delta_{T,0}},p_{\Delta_{T,0}}]} F[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}] \prod_{j=1}^{J} d\xi_j dx_j$$

$$\infty \times \infty \times \infty \times \infty \times \cdots\cdots\cdots, \quad J \to \infty$$

mathematically, we have only to add many assumptions.

- We have no assumption for $F[q,p] \in \mathcal{F}$ until this section.
- We will probably have at least one example $F[q,p] \equiv 1$

as the solution for the Schrödinger equation.

Do not consider other things.

- Then the class $\mathcal{F}$ will become large as a set.
- If lucky, $\mathcal{F}$ may contain other examples.

Since the oscillatory integral is defined by the integration by parts, we repeat the integration by parts for the multiple oscillatory integral.

We add ‘ $|\alpha_j|,\ |\beta_{j-1}| \le M$ ’ so that the multiple integral $(\star)$ can be controlled by

$$C \times C \times C \times C \times \cdots\cdots\cdots, \quad J \to \infty$$

Tentative Assumption Let $m \ge 0$. For any integer $M \ge 0$, there exist $A_M > 0$, $X_M > 0$ such that for any $|\alpha_j|,\ |\beta_{j-1}| \le M$, $j = 1, 2, \ldots, J, J+1$,

$$|(\prod_{j=1}^{J+1} \partial_{x_j}^{\alpha_j} \partial_{\xi_{j-1}}^{\beta_{j-1}}) F(x_{J+1}, \xi_J, \ldots, x_1, \xi_0, x_0)|$$

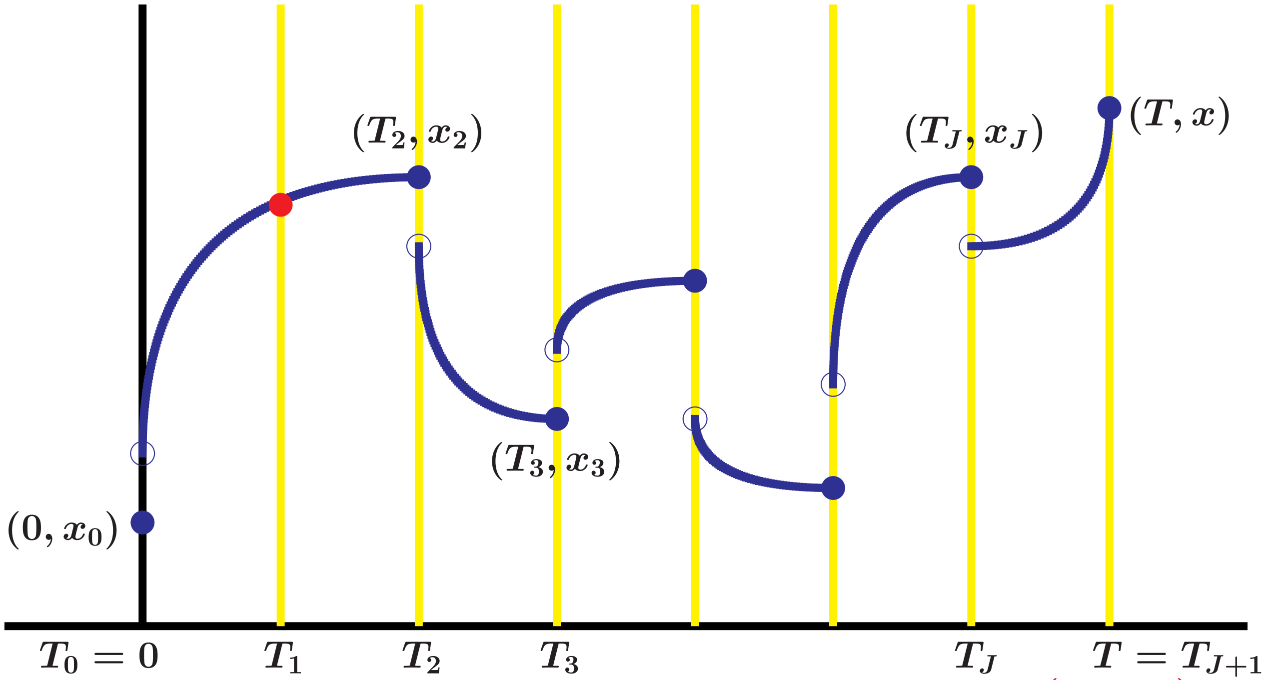
$$\le A_M (X_M)^{J+1} (1 + \sum_{j=1}^{J+1} (|x_j| + |\xi_{j-1}|) + |x_0|)^m.$$

By the stationary phase method, the main term of integral with respect to (ξ_1, x_1) implies the division $T = T_{J+1} > T_J > \cdots > T_2 > T_0 = 0$, i.e.,

$$\left(\frac{1}{2\pi\hbar}\right)^{d/2} \int_{R^{2d}} e^{\frac{i}{\hbar}\phi[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}]} F[q_{\Delta_{T,0}}, p_{\Delta_{T,0}}] d\xi_1 dx_1$$

$$= e^{\frac{i}{\hbar}\phi[q_{(\Delta_{T,T_2},0)}, p_{(\Delta_{T,T_2},0)}]} D_{T_2,T_1,0}(x_2, \xi_0)^{-1/2} F[q_{(\Delta_{T,T_2},0)}, p_{(\Delta_{T,T_2},0)}] + \hbar(\text{Remainder}).$$

Repeating this process with respect to (ξ_2, x_2), . . . , (ξ_J, x_J), we get the main term $e^{\frac{i}{\hbar}\phi[q_{T,0}, p_{T,0}]} D_{\Delta_{T,0}}(x, \xi_0)^{-1/2} F[q_{T,0}, p_{T,0}]$ of Theorem 4.



The main term of integral with respect to (ξ_1, x_1)

Furthermore, we add ' any $\Delta_{T,0}$ ' and small terms ' t_j ' so that the multiple integral $(\star)$ can be controlled by

$$C, \qquad \text{independent of } J \to \infty.$$

Tentative Assumption Let $m \geq 0$. For any integer $M \geq 0$, there exist $A_M > 0$, $X_M > 0$ such that for any $\Delta_{T,0}$, any $|\alpha_j|, |\beta_{j-1}| \leq M$, $j = 1, 2, \dots, J, J+1$,

$$|(\prod_{j=1}^{J+1} \partial_{x_j}^{\alpha_j} \partial_{\xi_{j-1}}^{\beta_{j-1}}) F_{\Delta_{T,0}}(x_{J+1}, \xi_J, \dots, x_1, \xi_0, x_0)|$$
$$\leq A_M (X_M)^{J+1} (\prod_{j=1}^{J+1} (t_j)^{\min(|\beta_{j-1}|,1)}) (1 + \sum_{j=1}^{J+1} (|x_j| + |\xi_{j-1}|) + |x_0|)^m .$$

Remark Note that $q_{\Delta_{T,0}}(t) \approx x_j - t_j \xi_{j-1}$ when $T_{j-1} < t \leq T_j$.

I do not treat the example $F[q,p] = B(t, q(t), p(t))$ because I do not know how to have sharp $q(t)$ and $p(t)$ at the same time t.

At last, we add ' u_k ' for the difference with respect to the height $F[q,p]$ so that the multiple integral $(\star)$ becomes a Cauchy sequence. $\square$

Assumption of $F[q,p] \in \mathcal{F}$ Let $m \geq 0$, $u_j \geq 0$, $\sum_{j=1}^{J+1} u_j \leq U < \infty$. For any integer $M \geq 0$, there exist $A_M > 0$, $X_M > 0$ such that for any $\Delta_{T,0}$, any $|\alpha_j|$, $|\beta_{j-1}| \leq M$, $j = 1, 2, \ldots, J, J+1$ and any $1 \leq k \leq J$,

$$|(\prod_{j=1}^{J+1} \partial_{x_j}^{\alpha_j} \partial_{\xi_{j-1}}^{\beta_{j-1}}) F_{\Delta_{T,0}}(x_{J+1}, \xi_J, \ldots, x_1, \xi_0, x_0)|$$

$$\leq A_M (X_M)^{J+1} (\prod_{j=1}^{J+1} (t_j)^{\min(|\beta_{j-1}|,1)})(1 + \sum_{j=1}^{J+1}(|x_j| + |\xi_{j-1}|) + |x_0|)^m,$$

$$|(\prod_{j=1}^{J+1} \partial_{x_j}^{\alpha_j} \partial_{\xi_{j-1}}^{\beta_{j-1}}) \partial_{x_k} F_{\Delta_{T,0}}(x_{J+1}, \xi_J, \ldots, x_1, \xi_0, x_0)|$$

$$\leq A_M (X_M)^{J+1} u_k (\prod_{j \neq k} (t_j)^{\min(|\beta_{j-1}|,1)})(1 + \sum_{j=1}^{J+1}(|x_j| + |\xi_{j-1}|) + |x_0|)^m.$$