Inoue, A.
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ON A "HAMILTONIAN PATH-INTEGRAL" DERIVATION OF THE SCHRÖDINGER EQUATION

ATSUSHI INOUE

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1. Introduction

1.1. Problem and Results

We consider the following initial value problem of the Schrödinger equation with an external electro-magnetic potential on $\mathbb{R}^m$ from the point of view of "**Hamiltonian path-integral quantization**" in $L^2(\mathbb{R}^m)$. In other words, we construct a parametrix which exhibits clearly how quantities from the Hamiltonian (not Lagrangian) mechanics are related to quantum mechanics:

$$(1.1)\qquad \begin{cases} \dfrac{\hbar}{i}\dfrac{\partial u(t,x)}{\partial t} + \mathbb{H}\left(t,x,\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}\right)u(t,x) = 0, \\ u(0,x) = u(x) \end{cases}$$

with

$$(1.2)\qquad \mathbb{H}\left(t,x,\frac{\hbar}{i}\frac{\partial}{\partial x}\right) = \frac{1}{2M}\sum_{j=1}^{m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j} - eA_j(t,x)\right)^2 + \lambda V(t,x).$$

Here, M, e and λ are constants, $A(t,x) = (A_j(t,x))$ and $V(t,x)$ are real-valued smooth functions on $\mathbb{R}\times\mathbb{R}^m$. For the sake of notational simplicity, we put $M = e = \lambda = 1$ in this paper.

REMARK. In the following, we use Einstein's convention of summing up w.r.t. indeces.

The following assumptions on $A(t,x)$ and $V(t,x)$ are due to Yajima [18] and Fujiwara [6]:

(A) $A_j(t,x) \in C^\infty(\mathbb{R}\times\mathbb{R}^m)$, real-valued and there exists $\epsilon > 0$ such that

$$|\partial_x^\alpha B_{jk}(t,x)| \le C_\alpha(1+|x|)^{-1-\epsilon} \text{ for } |\alpha| \ge 1,$$
$$|\partial_x^\alpha A_j(t,x)| + |\partial_x^\alpha \partial_t A_j(t,x)| \le C_\alpha \text{ for } |\alpha| \ge 1$$

where

$$B_{jk}(t,x) = \frac{\partial A_k(t,x)}{\partial x_j} - \frac{\partial A_j(t,x)}{\partial x_k}.$$

(V) $V(t,x) \in C^\infty(\mathbb{R} \times \mathbb{R}^m)$, real-valued and for any compact interval I, there exists a constant $C_{\alpha I} > 0$ such that

$$\sup_{t \in I} |\partial_x^\alpha V(t,x)| \le C_{\alpha I} \ \text{ for } \ |\alpha| \ge 2.$$

REMARK. By above assumptions, for any $T > 0$ and α, β, there exists a constant $C_{\alpha\beta}$ such that

$$\sup_{|t| \le T} |\partial_x^\alpha \partial_\xi^\beta H(t,x,\xi)| \le C_{\alpha\beta}(1 + |x| + |\xi|)^{(2-|\alpha+\beta|)_+} \tag{1.3}$$

where for any $\gamma \in \mathbb{R}$, we put $\gamma_+ = \max(\gamma, 0)$.

Outline of the strategy of quantization:

(1) We get the complete symbol of $\mathbb{H}(t, x, -i\hbar\partial_x)$ denoted by $H(t,x,\xi)$ independent of $\hbar$, which is called the Hamiltonian function. Using this function, we formulate the Hamilton equation:

$$\begin{cases} \dot{x}(t) = \partial_\xi H(t, x(t), \xi(t)), \\ \dot{\xi}(t) = -\partial_x H(t, x(t), \xi(t)). \end{cases} \tag{1.4}$$

(2) Solving this equation under Assumptions (A) and (V), we construct a phase function $S(t,s,x,\xi)$ which satisfies

$$\text{(Hamilton-Jacobi equation)} \begin{cases} \partial_t S(t,s,x,\xi) + H(t,x,\partial_x S(t,s,x,\xi)) = 0, \\ S(s,s,x,\xi) = x \cdot \xi. \end{cases} \tag{1.5}$$

Putting

$$D(t,s,x,\xi) = \det\left(\partial^2_{x_j \xi_k} S(t,s,x,\xi)\right),$$

we have

$$\text{(continuity equation)} \begin{cases} \partial_t D(t,s,x,\xi) \\ \quad + \partial_{x_j}\left[D(t,s,x,\xi)\partial_{\xi_j} H(t,x,\partial_x S(t,s,x,\xi))\right] = 0, \\ D(s,s,x,\xi) = 1. \end{cases} \tag{1.6}$$

(3) We define a Fourier Integral Operator on $\mathbb{R}^m$ as

$$E(t,s)u(x) = c_m \int_{\mathbb{R}^m} d\xi\, D^{1/2}(t,s,x,\xi) e^{i\hbar^{-1}S(t,s,x,\xi)} \hat{u}(\xi) \tag{1.7}$$

where

$$\hat{u}(\xi) = c_m \int_{\mathbb{R}^m} dx\, e^{-i\hbar^{-1}x\cdot\xi} u(x) \text{ with } c_m = (2\pi\hbar)^{-m/2}.$$

We show that this operator gives not only a bounded operator on $L^2(\mathbb{R}^m)$, but also a good parametrix for (1.1) by virtue of (1.5) and (1.6) : Let Δ be a subdivision of (s,t) such that

$$\Delta : t_0 = s < t_1 < \cdots < t_{\ell-1} < t_\ell = t \text{ and } \delta(\Delta) = \max_{j=1,\cdots,\ell} |t_j - t_{j-1}|.$$

Putting

$$E(\Delta|t,s)u = E(t,t_{\ell-1})E(t_{\ell-1},t_{\ell-2})\cdots E(t_1,s),$$

we claim that $\{E(\Delta|t,s)\}$ forms a "Cauchy net" w.r.t. $\delta(\Delta) \to 0$ in $L^2(\mathbb{R}^m)$ when $u \in \mathcal{S}(\mathbb{R}^m)$ and that it converges to an evolutional operator $\mathbb{U}(t,s)$, which is, as a consequence, a fundamental solution of (1.1).

Therefore, we have the following:

Main Theorem . *Fix $T > 0$ arbitrarily. Under Assumptions* (A) and (V), *there exists a family of operators $\{\mathbb{U}(t,s)\,|\,t,s \in [-T,T]\}$ acting on $L^2(\mathbb{R}^m)$ with the following properties:*

1. *$\mathbb{U}(t,s)$ is a unitary operator on $L^2(\mathbb{R}^m)$ for each $t,s \in [-T,T]$.*
2. *For any $u \in L^2(\mathbb{R}^m)$, $\mathbb{U}(t,s)u$ is a $L^2(\mathbb{R}^m)$-valued continuous function in $t,s \in [-T,T]$ and it satisfies*

$$\begin{cases} \mathbb{U}(s,s)u = u \text{ for any } s \in \mathbb{R}, \\ \mathbb{U}(t_1,t_2)\mathbb{U}(t_2,t_3)u = \mathbb{U}(t_1,t_3)u \text{ for any } t_1,t_2,t_3 \in [-T,T]. \end{cases}$$

3. *If $u \in \mathcal{S}(\mathbb{R}^m)$, $\mathbb{U}(t,s)u$ is a $L^2(\mathbb{R}^m)$-valued differentiable function in $(t,s) \in \mathbb{R}^2$ and it belongs to $C^\infty(\mathbb{R}^m)$ for each $(t,s) \in \mathbb{R}^2$. Moreover, it satisfies*

$$\begin{cases} \dfrac{\hbar}{i}\dfrac{\partial}{\partial t}\mathbb{U}(t,s)u + \mathbb{H}\Big(t,x,\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}\Big)\mathbb{U}(t,s)u = 0, \\ \dfrac{\hbar}{i}\dfrac{\partial}{\partial s}\mathbb{U}(t,s)u - \mathbb{U}(t,s)\mathbb{H}\Big(s,x,\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}\Big)u = 0. \end{cases}$$

Corollary. *Under Assumptions* (A) and (V), *there exists a constant $C > 0$ independent of t,s for $|t|,|s| < T$ such that if $\delta(\Delta)$ is sufficiently small, we have*

$$\|E(\Delta|t,s) - \mathbb{U}(t,s)\| \le C\delta(\Delta). \tag{1.8}$$

1.2. Remarks

(1) In this note, we assume that A_j and V are smooth enough in order to clarify the procedure itself.
(2) Fujiwara [6, 7] constructed a fundamental solution of the Schrödinger equation when $A = 0$ and a potential V satisfies milder conditions than (V), that is,

(i) V is a real-valued measurable function of $(t, x) \in \mathbb{R} \times \mathbb{R}^m$. For any fixed $t \in \mathbb{R}$, $V(t, x)$ is smooth in $x \in \mathbb{R}^m$.

(ii) For any multi-index α with $|\alpha| \geq 2$, the non-negative measurable function of t defined by

$$M_\alpha(t) = \sup_{x \in \mathbb{R}^m} |\partial_x^\alpha V(t, x)| + \sup_{|x| \leq 1} |V(t, x)|$$

is essentially bounded on every compact interval of $\mathbb{R}$.
In [6, 7], he modifies mathematically a part of Feynman's heuristic argument to construct a "good parametrix" for (1.1) with $A = 0$. Fujiwara used the Lagrangian formulation without resorting to Fourier transformations, that is, instead of (1.7), he considered an integral transformation of the form

$$F(t, s)u(x) = \Big(\frac{1}{2\pi i\hbar(t-s)}\Big)^{m/2} \int_{\mathbb{R}^m} e^{i\hbar^{-1}S(t,s,x,y)} u(y)dy,$$

where $S(t, s, x, y)$ satisfies the Hamilton-Jacobi equation in the Lagrangian formulation. Afterwards, Kitada [11] and Kitada & Kumano-go [12] reformulated Fujiwara's result in the Hamiltonian scheme with a vector potential A of special form. But, Intissar [10] critisized the method employed by [11, 12] saying that their methods yield a non-controllable remainder term in order to obtain the pseudo-differential operator (=ΨDO) of Weyl type as the infinitesimal generator of that parametrix. Moreover, he proposed a complicated procedure which is seemingly far from the spirit of quantization. On the other hand, Yajima [18] constructed a fundamental solution under Assumtions (A) and (V) using the Lagrangian formulation. As he intends to construct a fundamental solution and he doesn't claim his process as quantization, therefore he may apply the gauge transformation freely to the given Schrödinger equation. (But as we want to claim our process as quantization, we can't use gauge transformations to reform the Schrödinger equation itself before quantization being performed.) Moreover, in [7] (when $A = 0$) and [18] (when A exists), they give the kernel representation of the evolution operator in the Lagrangian formulation,

$$\mathbb{U}(t, s)u(x) = \int_{\mathbb{R}^m} b(t, s, x, y) e^{i\hbar^{-1}S(t,s,x,y)} u(y)dy,$$

at least $|t - s|$ being small.

Now, we want to claim that after slightly modifying Kitada and Kumano-go's method, we may construct a Schrödinger equation by "Hamiltonian path-integral method" when the Hamiltonian function belongs to a certain class. In fact, under same conditions to the vector potential A in [18], the Fourier Integral Operator (=FIO), which has phase and amplitude functions derived from corresponding classical mechanics, gives a good parametrix of the problem of type (1.1). More precisely, its "infinitesimal generator" is represented by a Weyl type ΨDO with a controllable remainder term. Here, we use a composition formulas of FIO with Weyl type ΨDO. (Seemingly, these composition formulas are simple but new in the sense being not yet published explicitly.)
(3) This paper is the improved version of Inoue [8], where we have the estimate (1.8) only for a special class of $A_j(t,x)$. Due to K. Taniguchi [17], we have now the proof of the conjecture concerning a composition formula of FIOs, which we proposed in [8]. Therefore, we have the good estimate of the composition of certain FIOs, by which we have the operator norm convergence of $E(\Delta|t,s)$ as in the above corollary.
(4) We may regard these constructions as a mathematical procedure of quantization of certain Lagrangian or Hamiltonian functions (see, Feynman [4] and also Inoue & Maeda [9]) on Euclidean space (By the technical difficulty, we couldn't consider the quantization problem on a curved space).

1.3. Prerequisite

For reader's sake, we quote here the following notion from Kumano-go [13]:

DEFINITION 1.1. (amplitude function) A C^∞-function $a(\eta,y)$ on $\mathbb{R}^{2m}$ is said to be an amplitude function denoted by $a\in\mathfrak{A}^k_{\delta,\tau}(\mathbb{R}^{2m})$ ($0\le\delta<1$, $0\le\tau$, $-\infty<k<\infty$) if for α,β, there exists a constant $C_{\alpha\beta}$ such that

$$(1.9)\qquad |\partial_\eta^\alpha\partial_y^\beta a(\eta,y)|\le C_{\alpha\beta}\langle\eta\rangle^{k+\delta|\beta|}\langle y\rangle^\tau \text{ with } \langle\eta\rangle^2=1+|\eta|^2,\ \langle y\rangle^2=1+|y|^2.$$

Putting

$$\mathfrak{A}(\mathbb{R}^{2m})=\bigcup_{0\le\delta<1}\ \bigcup_{-\infty<k<\infty}\ \bigcup_{0\le\tau}\mathfrak{A}^k_{\delta,\tau}(\mathbb{R}^{2m})$$

and introducing semi-norms on $\mathfrak{A}(\mathbb{R}^{2m})$ by

$$|a|_\ell=\max_{|\alpha+\beta|\le\ell}\sup_{\eta,y}\left\{|\partial_\eta^\alpha\partial_y^\beta a(\eta,y)|\langle\eta\rangle^{-(k+\delta|\beta|)}\langle y\rangle^{-\tau}\right\},$$

we define a Fréchet structure on $\mathfrak{A}(\mathbb{R}^{2m})$.

From now on, we abbreviate the domain of integration unless there occurs confusion.

DEFINITION 1.2. (oscillatory integral) For $a \in \mathfrak{A}(\mathbb{R}^{2m})$, we define

$$\int d\eta dy\, e^{-i\hbar^{-1}y\cdot\eta}a(\eta,y) = \lim_{\epsilon\to 0}\int d\eta dy\, \chi(\epsilon y,\epsilon\eta)e^{-i\hbar^{-1}y\cdot\eta}a(\eta,y)$$

with $\chi(\eta,y)\in\mathcal{S}(\mathbb{R}^{2m})$ satisfying $\chi(0,0)=1$.

Remarking

$$\langle y\rangle^{-2\ell}\langle D^{\hbar}_{\eta}\rangle^{-2\ell}e^{-i\hbar^{-1}y\cdot\eta} = e^{-i\hbar^{-1}y\cdot\eta} \text{ with } D^{\hbar}_{\eta} = \frac{\hbar}{i}\partial_{\eta},\ \langle D^{\hbar}_{\eta}\rangle^2 = 1-\hbar^2\Delta_{\eta},$$

we have

Proposition 1.3. *For $a\in\mathfrak{A}^{n}_{\delta,\tau}(\mathbb{R}^{2m})$ and $-2\ell(1-\delta)+n<-m$, $-2\ell'+\tau<-m$, we have*

$$\int d\eta dy\, e^{-i\hbar^{-1}y\cdot\eta}a(\eta,y) = \int d\eta dy\, e^{-i\hbar^{-1}y\cdot\eta}\langle y\rangle^{-2\ell'}\langle D^{\hbar}_{\eta}\rangle^{-2\ell'}[\langle\eta\rangle^{-2\ell}\langle D^{\hbar}_{y}\rangle^{-2\ell}a(\eta,y)].$$

In the above, the integrand of the right hand side is absolutely integrable w.r.t. $d\eta dy$, while the left hand side is considered as the oscillatory integral.

REMARKS. (i) Following formulas will be frequently used below: For $u\in\mathcal{B}(\mathbb{R}^m)$, we have

(1.10) $$u(x) = c_m^2\int_{\mathbb{R}^{2m}} dyd\eta\, e^{-i\hbar^{-1}y\cdot\eta}u(x+y) = c_m^2\int_{\mathbb{R}^{2m}} dyd\eta\, e^{i\hbar^{-1}(x-y)\cdot\eta}u(y),$$

(1.11)
$$1 = c_m^2\int_{\mathbb{R}^{2m}} dyd\eta\, e^{i\hbar^{-1}(x-y)\cdot\eta},\quad \delta(x) = c_m\int_{\mathbb{R}^m} d\eta\, e^{i\hbar^{-1}x\cdot\eta} = c_m\int_{\mathbb{R}^m} d\eta\, e^{-i\hbar^{-1}x\cdot\eta},$$

where

$$\mathcal{B}(\mathbb{R}^m) = \{u\in C^{\infty}(\mathbb{R}^m)\,|\,\partial_x^{\alpha}u \text{ are bounded on } \mathbb{R}^m \text{ for any } |\alpha|\geq 0\}.$$

(ii) For $f\in\mathfrak{A}(\mathbb{R}^{2m})$ satisfying $\partial^2_{\eta_j\eta_k}f(y,\eta)=0$, that is, $f(y,\eta)=f(y,0)+\eta_j f_{\eta_j}(y,0)$, we have

(1.12) $$c_m^2\int_{\mathbb{R}^{2m}} d\eta dy\, e^{-i\hbar^{-1}y\cdot\eta}f(y,\eta) = f(0,0)+i\hbar\partial^2_{y_j\eta_j}f(0,0).$$

(iii) In the following, all integrals are interpreted as oscillatory one, if necessary.

1.3.1. Pseudo-differential operators (=ΨDOs)

DEFINITION 1.4. (symbol function) A C^∞-function $p(x,\xi)$ on $\mathbb{R}^{2m}$ is said to be a symbol function of order ℓ denoted by $p \in \mathfrak{S}^\ell$ if for α, β, there exists a constant $C_{\alpha\beta}$ such that

$$|\partial_\xi^\alpha \partial_x^\beta p(x,\xi)| \le C_{\alpha\beta}(1+|x|+|\xi|)^{(\ell-|\alpha+\beta|)_+}. \tag{1.13}$$

A symbol-function $p(x,\xi)$ is called classical and denoted by $p \in \mathfrak{S}^\ell_{cl}$ if w.r.t. ξ, $p(x,\xi)$ is a polynomial of degree ℓ.

For $P(x,\xi) \in \mathfrak{S}^\ell$, we define, as oscillatory integral, the (pseudo)-differential operators of order ℓ:

$$\hat{P}(x, D_x^\hbar)u(x) = c_m \int d\xi\, P(x,\xi) e^{i\hbar^{-1}x\cdot\xi}\hat{u}(\xi), \tag{1.14}$$

$$\hat{P}^W(x, D_x^\hbar)u(x) = c_m^2 \int d\xi dy\, P\Big(\frac{x+y}{2}, \xi\Big) e^{i\hbar^{-1}(x-y)\cdot\xi} u(y) \tag{1.15}$$

for $u \in \mathcal{S}(\mathbb{R}^m)$ with $D_x^\hbar = -i\hbar\partial_x$.

Proposition 1.5. *Let $H(t,x,\xi)$ be a function derived from $\mathbb{H}(t,x,-i\hbar\partial_x)$ in* (1.2) *by*

$$H(t,x,\xi) = e^{-i\hbar^{-1}x\cdot\xi}\mathbb{H}\Big(t,x,\frac{\hbar}{i}\frac{\partial}{\partial x}\Big)e^{i\hbar^{-1}x\cdot\xi}\Big|_{\hbar=0} = \frac{1}{2}(\xi_j - A_j(t,x))^2 + V(t,x). \tag{1.16}$$

Then,

(1) *$\hat{H}^W(t,x,D_x^\hbar)u(x)$ and $\hat{H}(t,x,D_x^\hbar)u(x)$ are well-defined for $u \in \mathcal{S}(\mathbb{R}^m)$ satisfying*

$$\begin{aligned} &\mathbb{H}(t,x,D_x^\hbar)u(x) = \hat{H}^W(t,x,D_x^\hbar)u(x), \\ &(\hat{H}^W(t,x,D_x^\hbar) - \hat{H}(t,x,D_x^\hbar))u(x) = -\frac{\hbar}{2i}\frac{\partial A_j(t,x)}{\partial x_j}u(x). \end{aligned} \tag{1.17}$$

Moreover, for $u \in \mathcal{S}(\mathbb{R}^m)$ and $\ell \in \mathbf{Z}_+$, we have

$$|||\hat{H}^W(t,x,D_x^\hbar)u|||_\ell \le C|||u|||_{\ell+2} \text{ and } |||\hat{H}(t,x,D_x^\hbar)u|||_\ell \le C|||u|||_{\ell+2}, \tag{1.18}$$

where

$$|||u|||_\ell^2 = \sum_{|\alpha|+k\le\ell} \|\langle x\rangle^k \partial_x^\alpha u(x)\|^2, \quad \|u\|^2 = \int dx\, |u(x)|^2.$$

(2) *We have*

$$\hat{H}^W(t,x,D_x^\hbar)u(x) = c_m \int d\xi\, H^\hbar(t,x,\xi) e^{i\hbar^{-1}x\cdot\xi}\hat{u}(\xi) \tag{1.19}$$

with

$$H^\hbar(t,x,\xi) = H(t,x,\xi) - \frac{\hbar}{2i}\frac{\partial A_j(t,x)}{\partial x_j}. \tag{1.20}$$

REMARK. We denote by Y_ℓ the closure of $\mathcal{S}(\mathbb{R}^m)$ w.r.t. $|||\cdot|||_\ell$.

1.3.2. Fourier Integral Operators (=FIOs)

DEFINITION 1.6. (phase function) (i) For $0 \le \kappa < 1$ and integer $\ell \ge 0$, we say that a real valued function $\phi \in \tilde{\mathfrak{P}}(\kappa,\ell)$ if $\phi(x,\xi) \in C^{\ell+2}(\mathbb{R}^{2m})$ satisfying

$$|J|_\ell = \sum_{|\alpha+\beta|\le\ell+2} \sup_{x,\xi} \left(|\partial_x^\beta \partial_\xi^\alpha J(x,\xi)|(1+|x|+|\xi|)^{-(2-|\alpha+\beta|)_+}\right) \le \kappa \tag{1.21}$$

where $J(x,\xi) = \phi(x,\xi) - x\cdot\xi$. We introduce also

$$|J|_{2,\ell} = \sum_{2\le|\alpha+\beta|\le\ell+2} \sup_{x,\xi} |\partial_x^\beta \partial_\xi^\alpha J(x,\xi)|. \tag{1.22}$$

(ii) We put

$$\mathfrak{P}(\kappa,\ell) = \tilde{\mathfrak{P}}(\kappa,\ell) \cap \mathcal{B}^{2,\infty}(\mathbb{R}^{2m}) \text{ with}$$
$$\mathcal{B}^{k,\infty}(\mathbb{R}^{2m}) = \{\phi \in C^\infty(\mathbb{R}^{2m}) \mid \partial_x^\beta \partial_\xi^\alpha \phi \text{ are bounded on } \mathbb{R}^{2m} \text{ for } |\alpha+\beta| \ge k\}.$$

We consider the following integral operator:

(1.23)
$$F(\lambda, a_1, \cdots, a_k, \phi)u(x) = c_m \int d\xi\, a_1(\lambda,x,\xi)\cdots a_k(\lambda,x,\xi) e^{i\hbar^{-1}\phi(\lambda,x,\xi)}\hat{u}(\xi),$$

where $\lambda \in \Lambda$ with Λ being a fixed set in $\mathbb{R}$. Let $k \ge 1$ and let $\ell = (\ell_1,\cdots,\ell_k)$ be a multi-index with $|\ell| = \sum_{j=1}^k \ell_j$ and put $M = 2([n/2]+[5n/4]+2)+2|\ell|+\max_{1\le j\le k}\ell_j$.

We assume

(Aϕ) 1. $\phi(\lambda,x,\xi)$ is real valued and $\phi(\lambda,\cdot,\cdot) \in C^{M+1}(\mathbb{R}^m \times \mathbb{R}^m)$ for any $\lambda \in \Lambda$.

2. $\sup |\partial_x \partial_\xi \phi(\lambda, x, \xi) - I| < 1$.
3. $\sup_{\substack{3 \le |\alpha+\beta| \le M+2 \\ |\beta| \ge 1}} |\partial_x^\alpha \partial_\xi^\beta \phi(\lambda, x, \xi)| < \infty$

(Aa) 1. $a_j \in C^M(\mathbb{R}^m \times \mathbb{R}^m)$.
2. $\sup_{\ell_j \le |\alpha+\beta| \le M} |\partial_x^\alpha \partial_\xi^\beta a_j(\lambda, x, \xi)| < \infty$.

Lemma 1.7. (Kitada) *Define a map*

$$\mathbb{R}^m \ni x \to y(\lambda, x, \xi, \eta) = \int_0^1 d\tau \phi_\xi(\lambda, x, (1-\tau)\eta + \tau\xi) \in \mathbb{R}^m.$$

Then, under assumptions above, there exists an inverse map

$$\mathbb{R}^m \ni y \to z(\lambda, y, \xi, \eta) \in \mathbb{R}^m$$

satisfying

$$y = y(\lambda, z(\lambda, y, \xi, \eta), \xi, \eta), \quad x = z(\lambda, y(\lambda, x, \xi, \eta), \xi, \eta).$$

Proposition 1.8. (Kitada) *Let $a_j (j = 1, \cdots, k)$ and ϕ as above. Then, for any $\hat{u} \in C_0^\infty(\mathbb{R}_\xi^m)$, we have*

$$\|F(a, \phi)u\| \le K_\lambda \| \! |u| \! \|_{|\ell|} \tag{1.24}$$

with

$$K_\lambda = C_{n,k,\ell} \prod_{j=1}^k D_j (1 + |z(\lambda, 0, 0, 0)|)^{|\ell|},$$
$$D_j = \sup_{\ell_j \le |\alpha+\beta| \le M} |\partial_x^\alpha \partial_\xi^\beta a_j(\lambda, x, \xi)| + \sup_{|\alpha+\beta| < \ell_j} |\partial_x^\alpha \partial_\xi^\beta a_j(\lambda, 0, 0)|.$$

2. Classical mechanics corresponding to (1.1)

2.1. Hamiltonian flows

For the function $H(t,x,\xi)$ defined in (1.16), we want to construct a solution $(x(\tau), \xi(\tau))$ of

$$\begin{cases} \dfrac{d}{d\tau} x_j(\tau) = \partial_{\xi_j} H(\tau, x(\tau), \xi(\tau)) = \xi_j(\tau) - A_j(\tau, x(\tau)), \\ \dfrac{d}{d\tau} \xi_j(\tau) = -\partial_{x_j} H(\tau, x(\tau), \xi(\tau)) \\ \qquad = (\xi_k(\tau) - A_k(\tau, x(\tau)))\partial_{x_j} A_k(\tau, x(\tau)) - \partial_{x_j} V(\tau, x(\tau)), \end{cases} \tag{2.1}$$

with the initial condition at $\tau = s$ given by

$$(x(s), \xi(s)) = (\underline{x}, \underline{\xi}) \in \mathbb{R}^{2m}. \tag{2.2}$$

In order to use the anti-symmetry of B_{jk}, we use Lagrangian reformulation of (2.1) (see [18]). That is, putting $(q(\tau), v(\tau)) = (x(\tau), \xi(\tau) - A(\tau, x(\tau)))$, we consider

$$\begin{cases} \dfrac{d}{d\tau} q_j(\tau) = v_j(\tau), \\ \dfrac{d}{d\tau} v_j(\tau) = B_{jk}(\tau, q(\tau)) v_k(\tau) - \partial_t A_j(\tau, q(\tau)) - \partial_{x_j} V(\tau, q(\tau)), \end{cases} \tag{2.3}$$

with the initial data

$$(q(s), v(s)) = (\underline{x}, \underline{\zeta}), \ \underline{\zeta} = \underline{\xi} - A(s, \underline{x}). \tag{2.4}$$

REMARK. Above problem (2.1) was treated in [10, 11] only when $A_j(t, q) = a_{jk}(t) q_k$ in (1.2).

Following propositions in this subsection are amalgam of results in [6], [11], [12], [18].

Proposition 2.1. *Let $H(t, x, \xi)$ be given as* (1.16). *Under Assumptions* (A) and (V), *for any $(\tau, s) \in \mathbb{R}^2$ satisfying $|\tau - s| \le 1$, there exists a unique solution of* (2.3) *with* (2.4) *which is denoted by $q(\tau)$, $q(\tau, s)$, $q(\tau, s, \underline{x}, \underline{\zeta})$, $v(\tau), \cdots$, etc., depending on the context.*

Moreover, the solution $(q(\tau), v(\tau))$ of (2.3) *is smooth in $(\tau, s, \underline{x}, \underline{\zeta})$. Furthermore, if $|\tau - s| \le 1$ and $|\alpha + \beta| \ge 1$, there exist constants C and $C_{\alpha\beta}$ such that*

$$\begin{cases} |q(\tau, s, \underline{x}, \underline{\zeta}) - \underline{x} - (\tau - s)\underline{\zeta}| \le C(1 + |\underline{x}| + |\underline{\zeta}|)|\tau - s|^2, \\ |v(\tau, s, \underline{x}, \underline{\zeta}) - \underline{\zeta}| \le C(1 + |\underline{x}| + |\underline{\zeta}|)|\tau - s|, \\ \left|\partial_{\underline{x}}^{\alpha} \partial_{\underline{\zeta}}^{\beta} \left[q(\tau, s, \underline{x}, \underline{\zeta}) - \underline{x} - (\tau - s)\underline{\zeta}\right]\right| \le C_{\alpha\beta} |\tau - s|^{|\beta|+1}, \\ \left|\partial_{\underline{x}}^{\alpha} \partial_{\underline{\zeta}}^{\beta} \left[v(\tau, s, \underline{x}, \underline{\zeta}) - \underline{\zeta}\right]\right| \le C_{\alpha\beta} |\tau - s|^{|\beta|}. \end{cases} \tag{2.5}$$

Proof. Use $|V_{x_j}(x)| \le C\langle x \rangle$ which follows from Assumption (V). See, Lemma 2.1 and Proposition 2.2 of [18], and also Proposition 1.3 of [6]. Here, we used the fact $B_{jk} v_j v_k = 0$. □

Theorem 2.2. *Under Assumptions* (A) and (V), *for any* $(\tau, s) \in \mathbb{R}^2$ *satisfying* $|\tau - s| \le 1$, *there exists a unique solution of* (2.1) *with any initial data* $(\underline{x}, \underline{\xi}) \in \mathbb{R}^{2m}$, *which is represented by*

$$\text{(2.6)} \qquad \begin{cases} x(\tau, s, \underline{x}, \underline{\xi}) = q(\tau, s, \underline{x}, \underline{\xi} - A(s, \underline{x})), \\ \xi(\tau, s, \underline{x}, \underline{\xi}) = v(\tau, s, \underline{x}, \underline{\xi} - A(s, \underline{x})) + A(\tau, q(\tau, s, \underline{x}, \underline{\xi} - A(s, \underline{x}))). \end{cases}$$

Moreover, $(x(\tau, s, \underline{x}, \underline{\xi}), \xi(\tau, s, \underline{x}, \underline{\xi}))$ *are smooth in* $(\tau, s, \underline{x}, \underline{\xi})$ *for* $|\tau - s| \le 1$ *and satisfy the following estimates: For any* α, β, *there exists a constant* $C_{\alpha\beta}$ *such that*

$$\text{(2.7)} \qquad \begin{cases} |\partial_{\underline{x}}^{\alpha} \partial_{\underline{\xi}}^{\beta} (x(\tau, s, \underline{x}, \underline{\xi}) - \underline{x})| \le C_{\alpha\beta} |\tau - s| (1 + |\underline{x}| + |\underline{\xi}|)^{(1 - |\alpha + \beta|)_+}, \\ |\partial_{\underline{x}}^{\alpha} \partial_{\underline{\xi}}^{\beta} (\xi(\tau, s, \underline{x}, \underline{\xi}) - \underline{\xi})| \le C_{\alpha\beta} |\tau - s| (1 + |\underline{x}| + |\underline{\xi}|)^{(1 - |\alpha + \beta|)_+}. \end{cases}$$

Proof. By induction w.r.t. the order $|\alpha + \beta|$ of differentiation $\partial_{\underline{x}}^{\alpha} \partial_{\underline{\xi}}^{\beta}$, we get estimates (2.7) from (2.5) directly. See also, Proposition 2.3′ of [18]. □

Proposition 2.3. *Under Assumptions* (A) and (V), *there exists a constant* $0 < \delta_1 \le 1$ *such that, for any* $(t, s) \in \mathbb{R}^2$ *satisfying* $|t - s| < \delta_1$, *we have the following:*
(1) *For any fixed* $t, s, \underline{\xi}$, *the mapping*

$$\text{(2.8)} \qquad \mathbb{R}^m \ni \underline{x} \mapsto \bar{x} = x(t, s, \underline{x}, \underline{\xi}) \in \mathbb{R}^m$$

is a smooth-diffeomorphism. The inverse mapping

$$\text{(2.9)} \qquad \mathbb{R}^m \ni \bar{x} \mapsto \underline{x} = y(t, s, \bar{x}, \underline{\xi}) \in \mathbb{R}^m \textit{ satisfies} \quad \begin{cases} \bar{x} = x(t, s, y(t, s, \bar{x}, \underline{\xi}), \underline{\xi}) \text{ for any } (t, s, \bar{x}, \underline{\xi}), \\ \underline{x} = y(t, s, x(t, s, \underline{x}, \underline{\xi}), \underline{\xi}) \text{ for any } (t, s, \underline{x}, \underline{\xi}). \end{cases}$$

(2) *For any fixed* $t, s, \underline{x}$, *the mapping*

$$\text{(2.10)} \qquad \mathbb{R}^m \ni \underline{\xi} \mapsto \bar{\xi} = \xi(t, s, \underline{x}, \underline{\xi}) \in \mathbb{R}^m$$

is a smooth-diffeomorphism. The inverse mapping

$$\text{(2.11)} \qquad \mathbb{R}^m \ni \bar{\xi} \mapsto \underline{\xi} = \eta(t, s, \underline{x}, \bar{\xi}) \in \mathbb{R}^m \textit{ satisfies} \quad \begin{cases} \bar{\xi} = \xi(t, s, \underline{x}, \eta(t, s, \underline{x}, \bar{\xi})) \text{ for any } (t, s, \underline{x}, \bar{\xi}), \\ \underline{\xi} = \eta(t, s, \underline{x}, \xi(t, s, \underline{x}, \underline{\xi})) \text{ for any } (t, s, \underline{x}, \underline{\xi}). \end{cases}$$

(3) *By definition, we have*

$$(2.12)\qquad \begin{cases} x(s,s,\underline{x},\underline{\xi}) = \underline{x}, & \xi(s,s,\underline{x},\underline{\xi}) = \underline{\xi}, \\ y(t,t,\bar{x},\underline{\xi}) = \bar{x}, & \eta(t,t,\underline{x},\bar{\xi}) = \bar{\xi}. \end{cases}$$

(4) *Furthermore,* $(y(t),\eta(t))$ *is smooth in* (t,s,x,ξ) *with the following estimates: There exist constants* $C_{\alpha\beta}$*, independent of* (t,s,x,ξ)*, such that for any* α,β*,*

(2.13)
$$\begin{cases} |\partial_x^\alpha\partial_\xi^\beta(y(t,s,x,\xi)-x)| \le C_{\alpha\beta}|t-s|(1+|x|+|\xi|)^{(1-|\alpha+\beta|)_+} & (x=\bar{x},\ \xi=\underline{\xi}), \\ |\partial_x^\alpha\partial_\xi^\beta(\eta(t,s,x,\xi)-\xi)| \le C_{\alpha\beta}|t-s|(1+|x|+|\xi|)^{(1-|\alpha+\beta|)_+} & (x=\underline{x},\ \xi=\bar{\xi}). \end{cases}$$

Proof. Take δ_1 satisfying $C_{00}|t-s|<1$ where C_{00} is given in (2.7) of Theorem 2.2 and apply global implicit function theorem mentioned in [6]. Concerning estimates, see, Proposition 3.2 and 3.3 of [11]. □

2.2. The time reversing.

As we may solve (2.1) or (2.3) even if $s<t$ and t is the initial time, we consider the solution $x(\tau,t,\bar{x},\bar{\xi})$, $\xi(\tau,t,\bar{x},\bar{\xi})$, etc. of time reversed.

Then, we have

(2.14)
$$\begin{cases} \bar{x} = x(t,t,\bar{x},\bar{\xi}), & \underline{x} = x(s,t,\bar{x},\bar{\xi}), \\ \bar{\xi} = \xi(t,t,\bar{x},\bar{\xi}), & \underline{\xi} = \xi(s,t,\bar{x},\bar{\xi}), \end{cases} \quad \text{resp.} \quad \begin{cases} \bar{x} = x(t,s,\underline{x},\underline{\xi}), & \underline{x} = x(s,s,\underline{x},\underline{\xi}), \\ \bar{\xi} = \xi(t,s,\underline{x},\underline{\xi}), & \underline{\xi} = \xi(s,s,\underline{x},\underline{\xi}). \end{cases}$$

Analogously, for the inverse mappings, we have

(2.15)
$$\begin{cases} \bar{x} = y(s,t,\underline{x},\bar{\xi}), & \underline{x} = y(s,s,\underline{x},\bar{\xi}), \\ \bar{\xi} = \eta(s,t,\bar{x},\underline{\xi}), & \underline{\xi} = \eta(s,s,\bar{x},\underline{\xi}), \end{cases} \quad \text{resp.} \quad \begin{cases} \bar{x} = y(t,t,\bar{x},\underline{\xi}), & \underline{x} = y(t,s,\bar{x},\underline{\xi}), \\ \bar{\xi} = \eta(t,t,\underline{x},\bar{\xi}), & \underline{\xi} = \eta(t,s,\underline{x},\bar{\xi}). \end{cases}$$

Therefore, we have

(2.16)
$$\begin{cases} \eta(s,t,\bar{x},\underline{\xi}) = \xi(t,s,y(t,s,\bar{x},\underline{\xi}),\underline{\xi}), \\ y(s,t,\underline{x},\bar{\xi}) = x(t,s,\underline{x},\eta(t,s,\underline{x},\bar{\xi})), \end{cases} \quad \text{resp.} \quad \begin{cases} \eta(t,s,\underline{x},\bar{\xi}) = \xi(s,t,y(s,t,\underline{x},\bar{\xi}),\bar{\xi}), \\ y(t,s,\bar{x},\underline{\xi}) = x(s,t,\bar{x},\eta(s,t,\bar{x},\underline{\xi})). \end{cases}$$

By the uniqueness of the solution of (2.1), we have

$$\begin{cases} x(t,s,x(s,r,\underline{x},\underline{\xi}),\xi(s,r,\underline{x},\underline{\xi})) = x(t,r,\underline{x},\underline{\xi}), \\ \xi(t,s,x(s,r,\underline{x},\underline{\xi}),\xi(s,r,\underline{x},\underline{\xi})) = \xi(t,r,\underline{x},\underline{\xi}), \end{cases} \tag{2.17}$$

and also,

$$\begin{cases} x(r,s,x(s,t,\bar{x},\bar{\xi}),\xi(s,t,\bar{x},\bar{\xi})) = x(r,t,\bar{x},\bar{\xi}), \\ \xi(r,s,x(s,t,\bar{x},\bar{\xi}),\xi(s,t,\bar{x},\bar{\xi})) = \xi(r,t,\bar{x},\bar{\xi}). \end{cases} \tag{2.18}$$

By the same arguments of Theorem 2.2 and Proposition 2.3, we get

Proposition 2.4. *Under assumptions* (A), (V), *we have the following estimates:*

$$\begin{cases} |\partial_{\bar{x}}^{\alpha}\partial_{\bar{\xi}}^{\beta}(x(\tau,t,\bar{x},\bar{\xi})-\bar{x})| \le C_{\alpha\beta}|\tau-t|(1+|\bar{x}|+|\bar{\xi}|)^{(1-|\alpha+\beta|)_+}, \\ |\partial_{\bar{x}}^{\alpha}\partial_{\bar{\xi}}^{\beta}(\xi(\tau,t,\bar{x},\bar{\xi})-\bar{\xi})| \le C_{\alpha\beta}|\tau-t|(1+|\bar{x}|+|\bar{\xi}|)^{(1-|\alpha+\beta|)_+}. \end{cases} \tag{2.19}$$

Moreover,

(2.20)

$$\begin{cases} |\partial_{x}^{\alpha}\partial_{\xi}^{\beta}(y(s,t,x,\xi)-x)| \le C_{\alpha\beta}|t-s|(1+|x|+|\xi|)^{(1-|\alpha+\beta|)_+} \quad (x=\bar{x},\ \xi=\underline{\xi}), \\ |\partial_{x}^{\alpha}\partial_{\xi}^{\beta}(\eta(s,t,x,\xi)-\xi)| \le C_{\alpha\beta}|t-s|(1+|x|+|\xi|)^{(1-|\alpha+\beta|)_+} \quad (x=\underline{x},\ \xi=\bar{\xi}). \end{cases}$$

2.3. Action integral.

Define

$$S_0(t,s,\underline{x},\underline{\xi}) = \int_s^t \big[\dot{x}(\tau)\cdot\xi(\tau) - H(\tau,x(\tau),\xi(\tau))\big]d\tau \tag{2.21}$$

where $(x(\tau),\xi(\tau))$ are solutions of (2.1) with initial data $(\underline{x},\underline{\xi}) \in \mathbb{R}^{2m}$.

We put

$$\tilde{S}(t,s,\underline{x},\underline{\xi}) = \underline{x}\cdot\underline{\xi} + S_0(t,s,\underline{x},\underline{\xi}) \text{ with } \underline{x}\cdot\underline{\xi} = \underline{x}_j\underline{\xi}_j. \tag{2.22}$$

Using integration by parts, we get easily

$$\frac{\partial\tilde{S}(t,s,\underline{x},\underline{\xi})}{\partial\underline{x}_k} = \xi_\ell(t,s,\underline{x},\underline{\xi})\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial\underline{x}_k}, \tag{2.23}$$

$$\frac{\partial\tilde{S}(t,s,\underline{x},\underline{\xi})}{\partial\underline{\xi}_k} = \underline{x}_k + \xi_\ell(t,s,\underline{x},\underline{\xi})\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial\underline{\xi}_k}. \tag{2.24}$$

On the other hand, by the very definition of the inverse map (2.9), we have

$$\delta_{\ell j}=\frac{\partial\bar{x}_\ell}{\partial\bar{x}_j}=\Big[\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial\underline{x}_k}\frac{\partial y_k(t,s,\bar{x},\underline{\xi})}{\partial\bar{x}_j}\Big]\Big|_{\underline{x}=y(t,s,\bar{x},\underline{\xi})},\tag{2.25}$$

$$0=\frac{\partial\bar{x}_\ell}{\partial\underline{\xi}_j}=\Big[\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial\underline{x}_k}\frac{\partial y_k(t,s,\bar{x},\underline{\xi})}{\partial\underline{\xi}_j}+\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial\underline{\xi}_j}\Big]\Big|_{\underline{x}=y(t,s,\bar{x},\underline{\xi})}.\tag{2.26}$$

Putting

$$S(t,s,\bar{x},\underline{\xi})=\tilde{S}(t,s,y(t,s,\bar{x},\underline{\xi}),\underline{\xi}),\tag{2.27}$$

we have:

Proposition 2.5. (Hamilton-Jacobi equation) *If* $|t-s|<\delta_1$, *then* $S(t,s,\bar{x},\underline{\xi})$ *is smooth in* $(t,s,\bar{x},\underline{\xi})$ *and it satisfies the following:*

$$S(s,s,\bar{x},\underline{\xi})=\bar{x}\cdot\underline{\xi}.\tag{2.28}$$

$$\begin{cases}\partial_t S(t,s,\bar{x},\underline{\xi})+H(t,\bar{x},\partial_{\bar{x}}S(t,s,\bar{x},\underline{\xi}))=0,\\ \partial_s S(t,s,\bar{x},\underline{\xi})-H(s,\partial_{\underline{\xi}}S(t,s,\bar{x},\underline{\xi}),\underline{\xi})=0.\end{cases}\tag{2.29}$$

$$\partial_{\bar{x}_j}S(t,s,\bar{x},\underline{\xi})=\eta_j(s,t,\bar{x},\underline{\xi}),\quad \partial_{\underline{\xi}_j}S(t,s,\bar{x},\underline{\xi})=y_j(t,s,\bar{x},\underline{\xi}).\tag{2.30}$$

Moreover, $S(t,s,\bar{x},\underline{\xi})$ *satisfies the following estimates:*

(2.31)
$$|\partial_{\bar{x}}^\alpha\partial_{\underline{\xi}}^\beta(S(t,s,\bar{x},\underline{\xi})-\bar{x}\cdot\underline{\xi})|\le C_{\alpha\beta}|t-s|(1+|\bar{x}|+|\underline{\xi}|)^{(2-|\alpha+\beta|)_+}\ \text{for any}\ \alpha,\ \beta,$$

$$|S(t',s',\bar{x},\underline{\xi})-S(t,s,\bar{x},\underline{\xi})|\le C(1+|\bar{x}|+|\underline{\xi}|)^2(|t-t'|+|s-s'|).\tag{2.32}$$

Proof. For the future use, we give an elementary proof of (2.29) and (2.30). By the definition (2.27), (2.23), (2.25) and (2.16), we get

$$\begin{aligned}S_{\bar{x}_j}(t,s,\bar{x},\underline{\xi})&=\tilde{S}_{\underline{x}_k}(t,s,y(t,s,\bar{x},\underline{\xi}),\underline{\xi})\frac{\partial y_k(t,s,\bar{x},\underline{\xi})}{\partial\bar{x}_j}\\&=\Big[\xi_\ell(t,s,\underline{x},\underline{\xi})\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial\underline{x}_k}\Big]\Big|_{\underline{x}=y(t,s,\bar{x},\underline{\xi})}\cdot\frac{\partial y_k(t,s,\bar{x},\underline{\xi})}{\partial\bar{x}_j}\\&=\xi_j(t,s,y(t,s,\bar{x},\underline{\xi}),\underline{\xi})=\eta_j(s,t,\bar{x},\underline{\xi}).\end{aligned}$$

Using (2.27), (2.23), (2.24) and (2.26), we have

$$
\begin{aligned}
S_{\underline{\xi}_j}(t,s,\bar{x},\underline{\xi}) &= \Big[\tilde{S}_{\underline{x}_k}(t,s,\underline{x},\underline{\xi})\frac{\partial y_k(t,s,\bar{x},\underline{\xi})}{\partial \underline{\xi}_j} + \tilde{S}_{\underline{\xi}_j}(t,s,\underline{x},\underline{\xi})\Big]\Big|_{\underline{x}=y(t,s,\bar{x},\underline{\xi})} \\
&= \Big[\xi_\ell(t,s,\underline{x},\underline{\xi})\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial \underline{x}_k}\frac{\partial y_k(t,s,\bar{x},\underline{\xi})}{\partial \underline{\xi}_j}\Big]\Big|_{\underline{x}=y(t,s,\bar{x},\underline{\xi})} \\
&+ \Big[\underline{x}_j + \xi_\ell(t,s,\underline{x},\underline{\xi})\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial \underline{\xi}_j}\Big]\Big|_{\underline{x}=y(t,s,\bar{x},\underline{\xi})} \\
&= y_j(t,s,\bar{x},\underline{\xi}) \\
&+ \Big[\xi_\ell(t,s,\underline{x},\underline{\xi})\Big(\frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial \underline{\xi}_j} + \frac{\partial x_\ell(t,s,\underline{x},\underline{\xi})}{\partial \underline{x}_k}\frac{\partial y_k(t,s,\bar{x},\underline{\xi})}{\partial \underline{\xi}_j}\Big)\Big]\Big|_{\underline{x}=y(t,s,\bar{x},\underline{\xi})} \\
&= y_j(t,s,\bar{x},\underline{\xi}).
\end{aligned}
$$

By these, (2.30) is proved.

Remarking $S(t,s,x(t,s,\underline{x},\underline{\xi}),\underline{\xi}) = \tilde{S}(t,s,\underline{x},\underline{\xi})$ by (2.27), using (2.9) and (2.22), we have

$$
\begin{aligned}
&\dot{x}_k(t,s,\underline{x},\underline{\xi})\xi_k(t,s,\underline{x},\underline{\xi}) - H(t,x(t,s,\underline{x},\underline{\xi}),\xi(t,s,\underline{x},\underline{\xi})) = \frac{\partial \tilde{S}}{\partial t}(t,s,\underline{x},\underline{\xi}) \\
&= S_t(t,s,x(t,s,\underline{x},\underline{\xi}),\underline{\xi}) + S_{\bar{x}_j}(t,s,x(t,s,\underline{x},\underline{\xi}),\underline{\xi})\frac{\partial x_j(t,s,\underline{x},\underline{\xi})}{\partial t}.
\end{aligned}
$$

As we have

$$
\begin{aligned}
S_{\bar{x}_j}(t,s,x(t,s,\underline{x},\underline{\xi}),\underline{\xi}) = \xi_j(t,s,\underline{x},\underline{\xi}),\ H(t,x(t,s,\underline{x},\underline{\xi}),\xi(t,s,\underline{x},\underline{\xi}))\big|_{\underline{x}=y(t,s,\bar{x},\underline{\xi})} \\
= H(t,\bar{x},\partial_{\bar{x}}S(t,s,\bar{x},\underline{\xi})),
\end{aligned}
$$

we get the first equation of (2.29).

Using the integration by parts and (2.1), we get

$$
\begin{aligned}
\frac{\partial \tilde{S}}{\partial s}(t,s,\underline{x},\underline{\xi}) &= -\dot{x}(s,s,\underline{x},\underline{\xi})\cdot\underline{\xi} + H(s,\underline{x},\underline{\xi}) \\
&+ \int_s^t d\tau\Big[\frac{\partial \dot{x}_k(\tau,s)}{\partial s}\xi_k(\tau,s) - H_{x_k}(\tau,x(\tau,s),\xi(\tau,s))\frac{\partial x_k(\tau,s)}{\partial s}\Big] \\
&= -\dot{x}(s,s,\underline{x},\underline{\xi})\cdot\underline{\xi} + H(s,\underline{x},\underline{\xi}) + \frac{\partial x(t,s)}{\partial s}\cdot\xi(t,s,\underline{x},\underline{\xi}) - \frac{\partial x(t,s)}{\partial s}\Big|_{t=s}\cdot\underline{\xi}.
\end{aligned}
$$

On the other hand, differentiating $S(t,s,x(t,s,\underline{x},\underline{\xi}),\underline{\xi}) = \tilde{S}(t,s,\underline{x},\underline{\xi})$ w.r.t. s, we have

$$-\dot{x}(s,s,\underline{x},\underline{\xi})\cdot\underline{\xi} + H(s,\underline{x},\underline{\xi}) + \frac{\partial x(t,s)}{\partial s}\cdot\xi(t,s,\underline{x},\underline{\xi}) - \frac{\partial x(t,s)}{\partial s}\bigg|_{t=s}\cdot\underline{\xi}$$
$$= S_s(t,s,x(t,s,\underline{x},\underline{\xi}),\underline{\xi}) + S_{\bar{x}_j}(t,s,x(t,s,\underline{x},\underline{\xi}),\underline{\xi})\frac{\partial x_j(t,s,\underline{x},\underline{\xi})}{\partial s}.$$

As we have, by differentiating $\underline{x} = x(s,s,\underline{x},\underline{\xi})$ w.r.t. s,

$$0 = \dot{x}(s,s,\underline{x},\underline{\xi}) + \frac{\partial x(t,s,\underline{x},\underline{\xi})}{\partial s}\bigg|_{t=s},$$

we get

$$S_s(t,s,x(t,s,\underline{x},\underline{\xi}),\underline{\xi}) - H(s,\underline{x},\underline{\xi}) = 0,$$

that is, substituting $\underline{x} = y(t,s,\bar{x},\underline{\xi})$ and using the second relation in (2.30), we get the second equation of (2.29).

If $|\alpha+\beta|\geq 1$, $\partial_{\bar{x}}^{\alpha}\partial_{\underline{\xi}}^{\beta}(S(t,s,\bar{x},\underline{\xi})-\bar{x}\cdot\underline{\xi})$ is estimated as (2.31) by combining (2.30) and (2.20). Using this, (1.3) and (2.29), we have easily

$$|S(t,s,\bar{x},\underline{\xi}) - \bar{x}\cdot\underline{\xi}| \leq \int_s^t d\tau \left|H(\tau,\bar{x},\partial_x S(\tau,s,\bar{x},\underline{\xi}))\right| \leq C|t-s|(1+|\bar{x}|+|\underline{\xi}|)^2.$$

(2.32) is obtained with (2.31) from

$$S(t',s',\bar{x},\underline{\xi}) - S(t,s,\bar{x},\underline{\xi}) = \int_0^1 d\theta[(t'-t)S_t + (s'-s)S_s](\theta t' + (1-\theta)t, \theta s' + (1-\theta)s, \bar{x}, \underline{\xi}).$$

See also, Proposition 3.2 and 3.5 in [11]. □

2.4. Continuity equation.

Put

$$D(t,s,\bar{x},\underline{\xi}) = \det\left(\frac{\partial^2 S(t,s,\bar{x},\underline{\xi})}{\partial\bar{x}_k\partial\underline{\xi}_j}\right) = \det\left(\frac{\partial y_j(t,s,\bar{x},\underline{\xi})}{\partial\bar{x}_k}\right), \tag{2.33}$$

which is well-defined for $(t,s)\in\mathbb{R}^2$ satisfying $|t-s|\leq\delta_1$, because of Proposition 2.5.

Proposition 2.6. (Continuity equation) *Let Assumptions* (A) and (V) *hold, then* $D(t,s,\bar{x},\underline{\xi})$ *satisfies the following equation for* $|t-s|\leq\delta_1$*:*

$$D(s,s,\bar{x},\underline{\xi}) = 1. \tag{2.34}$$

$$(2.35)\qquad \begin{cases} \partial_t D(t,s,\bar{x},\underline{\xi}) + \partial_{\bar{x}_j}\left[D(t,s,\bar{x},\underline{\xi})\partial_{\xi_j} H(t,\bar{x},\partial_{\bar{x}} S(t,s,\bar{x},\underline{\xi}))\right] = 0, \\ \partial_s D(t,s,\bar{x},\underline{\xi}) - \partial_{\underline{\xi}_j}\left[D(t,s,\bar{x},\underline{\xi})\partial_{x_j} H(s,\partial_{\underline{\xi}} S(t,s,\bar{x},\underline{\xi}),\underline{\xi})\right] = 0. \end{cases}$$

Moreover, for any α, β, there exists a constant $C_{\alpha,\beta}$ independent of x, ξ and t, s with $|t-s| \le \delta_1$ such that

$$(2.36)\qquad |\partial_x^\alpha \partial_\xi^\beta (D(t,s,\bar{x},\underline{\xi}) - 1)| \le C_{\alpha\beta}|t-s|.$$

Proof. By differentiating the first equation of (2.29) w.r.t. $\underline{\xi}_j$, we get

$$\frac{\partial S_t}{\partial \underline{\xi}_j} + \frac{\partial S_{\bar{x}_\ell}}{\partial \underline{\xi}_j} H_{\xi_\ell} = 0 \ \text{ for } \ j,\ell = 1,\cdots,m.$$

Differentiating once more w.r.t. $\bar{x}_k$, we have

$$\frac{\partial^2 S_t}{\partial \bar{x}_k \partial \underline{\xi}_j} + \frac{\partial^2 S_{\bar{x}_\ell}}{\partial \bar{x}_k \partial \underline{\xi}_j} H_{\xi_\ell} + \frac{\partial^2 S}{\partial \underline{\xi}_j \partial \bar{x}_\ell}\frac{\partial H_{\xi_\ell}}{\partial \bar{x}_k} = 0.$$

Putting $S_{kj} = \partial^2 S / \partial \bar{x}_k \partial \underline{\xi}_j$ and rewriting above, we get

$$(2.37)\qquad \frac{\partial S_{kj}}{\partial t} + \frac{\partial S_{kj}}{\partial \bar{x}_\ell} H_{\xi_\ell} + S_{\ell j}\frac{\partial H_{\xi_\ell}}{\partial \bar{x}_k} = 0.$$

In general, for any invertible $m \times m$ matrix X depending on parameter τ, we have

$$(2.38)\qquad \frac{\partial}{\partial \tau}\det X = \operatorname{tr}(X^{-1}X_\tau)\det X = \det X \ \operatorname{tr}(X_\tau X^{-1}).$$

Here, we use the following convention:

$$\left(\frac{\partial X}{\partial \tau}\right)_{jk} = \frac{\partial X_{jk}}{\partial \tau}.$$

As $D = \det(S_{kj}) = \det S$ and using the second equality of (2.38), we have

$$D^{-1}\frac{\partial D}{\partial t} = S_{jk}^{-1}\frac{\partial S_{kj}}{\partial t}.$$

Remarking also

$$(2.39)\qquad S_{jk}^{-1}\frac{\partial S_{kj}}{\partial \bar{x}_\ell} = D^{-1}\frac{\partial D}{\partial \bar{x}_\ell}, \quad S_{jk}^{-1} S_{\ell j} = \delta_{\ell k},$$

and multiplying S^{-1}_{jk} to (2.37), we get

$$D^{-1}\frac{\partial D}{\partial t}+D^{-1}\frac{\partial D}{\partial \bar{x}_\ell}H_{\xi_\ell}+\frac{\partial H_{\xi_\ell}}{\partial \bar{x}_\ell}=0,$$

that is, we have the first equation in (2.35). The second one is also obtained by the same fashion. (This proof is essentially due to Mañes & Zumino [16].)

Estimates: By the definition of D and (2.31), we have easily

$$|\partial_x^\alpha \partial_\xi^\beta D(t,s,\bar{x},\underline{\xi})|\le C_{\alpha\beta}|t-s| \ \text{ for } \ |\alpha+\beta|\ge 1,\ |t-s|\le\delta_1\le 1. \tag{2.40}$$

Applying the method of characteristics to (2.35), we have the representation

$$D(t,s,\bar{x},\underline{\xi})=\exp\Big(-\int_s^t d\tau\big[H_{x_k\xi_k}(\tau)+S_{x_\ell x_k}(\tau)H_{\xi_\ell\xi_k}(\tau)\big]\Big) \tag{2.41}$$

where $H_*(\tau)=H_*(\tau,X(\tau),\eta(s,t,X(\tau),\underline{\xi}))$ and $S_*(\tau)=S_*(\tau,s,X(\tau),\underline{\xi})$, respectively. Here, we put $X(\tau)=x(\tau,s,y(t,s,\bar{x},\underline{\xi}),\underline{\xi})$, which is the solution of $\dfrac{dX_j(\tau)}{d\tau}=H_{\xi_j}(\tau,X(\tau),\eta(s,t,X(\tau),\underline{\xi}))$. Therefore, by (1.3), (2.31) and $D(t,s,\bar{x},\underline{\xi})-1=\displaystyle\int_s^t d\sigma\frac{d}{d\sigma}D(\sigma,s,\bar{x},\underline{\xi})$, we have

$$\begin{aligned}|D(t,s,\bar{x},\underline{\xi})-1|&\le\int_s^t d\sigma\big|H_{x_k\xi_k}(\sigma)+S_{x_\ell x_k}(\sigma)H_{\xi_\ell\xi_k}(\sigma)\big|\exp\Big(-\int_s^\sigma d\tau\big[H_{x_k\xi_k}(\tau)\\&\qquad\qquad+S_{x_\ell x_k}(\tau)H_{\xi_\ell\xi_k}(\tau)\big]\Big)\\&\le C|t-s|,\end{aligned}$$

since $|H_{x_k\xi_k}(\cdot)+S_{x_\ell x_k}(\cdot)H_{\xi_\ell\xi_k}(\cdot)|\le C$ and $|t-s|\le\delta_1\le 1$. This yields (2.36) with $\alpha+\beta=0$. □

Now, we put

$$\mu(t,s,\bar{x},\underline{\xi})=D^{1/2}(t,s,\bar{x},\underline{\xi}) \tag{2.42}$$

which is called the van Vleck determinant (see, [9]).
By using Proposition 2.6, we get easily the following:

Proposition 2.7. *For $|t-s|\le\delta_1$, $\mu(t,s,\bar{x},\underline{\xi})$ satisfies the following:*

$$\mu(s,s,\bar{x},\underline{\xi})=1. \tag{2.43}$$

$$\text{(2.44)}\quad \begin{cases} \partial_t\mu(t,s,\bar{x},\underline{\xi}) + \partial_{\bar{x}_j}\mu(t,s,\bar{x},\underline{\xi})\,\partial_{\xi_j}H(t,\bar{x},\partial_{\bar{x}}S(t,s,\bar{x},\underline{\xi})) \\ \qquad\qquad + \dfrac{1}{2}\mu(t,s,\bar{x},\underline{\xi})\partial_{\bar{x}_j}\big[\partial_{\xi_j}H(t,\bar{x},\partial_{\bar{x}}S(t,s,\bar{x},\underline{\xi}))\big] = 0, \\ \partial_s\mu(t,s,\bar{x},\underline{\xi}) - \partial_{\underline{\xi}_j}\mu(t,s,\bar{x},\underline{\xi})\,\partial_{x_j}H(s,\partial_{\underline{\xi}}S(t,s,\bar{x},\underline{\xi}),\underline{\xi}) \\ \qquad\qquad - \dfrac{1}{2}\mu(t,s,\bar{x},\underline{\xi})\partial_{\underline{\xi}_j}\big[\partial_{x_j}H(s,\partial_{\underline{\xi}}S(t,s,\bar{x},\underline{\xi}),\underline{\xi})\big] = 0. \end{cases}$$

Moreover, for any α,β, there exists a constant $C_{\alpha,\beta}$ independent of x,ξ and t,s with $|t-s|\le\delta_1$ such that

$$\text{(2.45)}\quad |\partial_x^\alpha\partial_\xi^\beta(\mu(t,s,\bar{x},\underline{\xi})-1)| \le C_{\alpha\beta}|t-s|.$$

3. Composition formulas for FIO with ΨDO

3.1. Composition of FIO with ΨDO from the left

We give some composition formulas of the operator $\hat{H}^W(x,D_x^\hbar)$ with FIO $F(a,\phi)$ defined by

$$\text{(3.1)}\quad F(a,\phi)u(x) = c_m\int_{\mathbb{R}^m} d\xi\, a(x,\xi)e^{i\hbar^{-1}\phi(x,\xi)}\hat{u}(\xi).$$

Theorem 3.1. *Let $F(a,\phi)$ be FIO defined by* (3.1) *with $\phi\in\mathfrak{P}$, $a\in\mathfrak{A}$. Let $\hat{H}^W(x,D_x^\hbar)$ be a Weyl type pseudo-differential operator with symbol $H(x,\xi)\in\mathfrak{S}^2(\mathbb{R}^{2m})$ given by* (1.16) *disregarding the time-dependence. Then, there exists $c_L=c_L(x,\eta)\in C^\infty(\mathbb{R}^{2m})$ such that*

$$\text{(3.2)}\quad \hat{H}^W(x,D_x^\hbar)F(a,\phi) = F(c_L,\phi).$$

Moreover, c_L has the following expansion

$$\text{(3.3)}\quad c_L = Ha - i\hbar\Big\{\partial_{\xi_j}H\cdot\partial_{x_j}a + \frac{1}{2}\Big(\partial^2_{x_j\xi_j}H + \partial^2_{x_jx_k}\phi\cdot\partial^2_{\xi_k\xi_j}H\Big)a\Big\} + r_L.$$

Here, the argument of H is $(x,\partial_x\phi(x,\eta))$ and that of ϕ and r_L is (x,η). Moreover, $r_L(x,\eta)\in C^\infty(\mathbb{R}^{2m})$ is given by

$$\text{(3.4)}\quad r_L(x,\eta) = -\frac{\hbar^2}{2}\partial^2_{\xi_k\xi_j}H(x,\partial_x\phi(x,\eta))\,\partial^2_{x_jx_k}a(x,\eta).$$

Proof. By definition, we have

(3.5)

$$\hat{H}^W(x,D_x^\hbar)F(a,\phi)u(x) = c_m^3\int d\xi\,dy\,d\eta\,H\Big(\frac{x+y}{2},\xi\Big)a(y,\eta)e^{i\hbar^{-1}((x-y)\cdot\xi+\phi(y,\eta))}\hat{u}(\eta)$$
$$= c_m\int d\eta\,c_L(x,\eta)e^{i\hbar^{-1}\phi(x,\eta)}\hat{u}(\eta).$$

Here, we put

$$c_L(x,\eta) = c_m^2\int d\xi\,dy\,q(x,\xi,y,\eta)e^{i\hbar^{-1}\psi(x,\xi,y,\eta)} \tag{3.6}$$

with

$$\psi(x,\xi,y,\eta)=(x-y)\cdot\xi+\phi(y,\eta)-\phi(x,\eta) \text{ and } q(x,\xi,y,\eta)=H\Big(\frac{x+y}{2},\xi\Big)a(y,\eta).$$

(I) Before giving the full proof, we calculate rather formally which yields (3.3). As

$$\phi(y,\eta)-\phi(x,\eta) = (y_j-x_j)\widetilde{\partial_{x_j}\phi}(x,y-x,\eta) = (y-x)\cdot\widetilde{\partial_x\phi}(x,y-x,\eta) \tag{3.7}$$

where

$$\widetilde{\partial_{x_j}\phi}(x,y-x,\eta) = \int_0^1 d\tau\,\partial_{x_j}\phi(x+\tau(y-x),\eta),$$

we introduce a change of variables by

$$\begin{cases} \tilde{y}=y-x, \\ \tilde{\xi}=\xi-\widetilde{\partial_x\phi}(x,y-x,\eta), \end{cases} \longleftrightarrow \begin{cases} y=\tilde{y}+x, \\ \xi=\tilde{\xi}+\widetilde{\partial_x\phi}(x,\tilde{y},\eta). \end{cases} \tag{3.8}$$

Inserting these into (3.6), we get

$$c_L(x,\eta) = c_m^2\int d\tilde{\xi}d\tilde{y}\,e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\xi}}H\Big(x+\frac{\tilde{y}}{2},\tilde{\xi}+\widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big)a(x+\tilde{y},\eta). \tag{3.9}$$

By Taylor's formula w.r.t. $\tilde{\xi}$, we have

(3.10)

$$H\Big(x+\frac{\tilde{y}}{2},\tilde{\xi}+\widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big)=H\Big(x+\frac{\tilde{y}}{2},\widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big)+\tilde{\xi}_j\partial_{\xi_j}H\Big(x+\frac{\tilde{y}}{2},\widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big)$$
$$+\tilde{\xi}_j\tilde{\xi}_k\int_0^1 d\tau_1(1-\tau_1)\partial^2_{\xi_j\xi_k}H\Big(x+\frac{\tilde{y}}{2},\tau_1\tilde{\xi}+\widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big).$$

Using (1.11), we get easily that

(3.11)
$$c_m^2 \int d\tilde{y}d\tilde{\xi}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\xi}} H\Big(x+\frac{\tilde{y}}{2}, \widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big) a(x+\tilde{y},\eta) = H(x,\partial_x\phi(x,\eta))a(x,\eta).$$

On the other hand, remarking $\tilde{\xi}_j\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\xi}} = i\hbar\partial_{\tilde{y}_j} e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\xi}}$ and applying (1.11) after integration by parts, we have

(3.12)
$$\begin{aligned}
&c_m^2 \int d\tilde{y}d\tilde{\xi}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\xi}}\tilde{\xi}_j\partial_{\xi_j} H\Big(x+\frac{\tilde{y}}{2}, \widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big) a(x+\tilde{y},\eta) \\
&\quad = -i\hbar c_m^2 \int d\tilde{y}d\tilde{\xi}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\xi}}\partial_{\tilde{y}_j}\Big[\partial_{\xi_j} H\Big(x+\frac{\tilde{y}}{2}, \widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big) a(x+\tilde{y},\eta)\Big] \\
&\quad = -i\hbar\partial_{\tilde{y}_j}\Big[\partial_{\xi_j} H\Big(x+\frac{\tilde{y}}{2}, \widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big) a(x+\tilde{y},\eta)\Big]\Big|_{\tilde{y}=0} \\
&\quad = -i\hbar\Big\{\partial_{\xi_j} H\,\partial_{x_j}a + \frac{1}{2}\Big(\partial^2_{x_j\xi_j}H + \partial^2_{x_jx_k}\phi\,\partial^2_{\xi_k\xi_j}H\Big)a\Big\}.
\end{aligned}$$

Thus, we get the main terms of (3.3) formally.

The remainder term is derived from

(3.13)
$$\begin{aligned}
r_L(x,\eta) = c_m^2 \int d\tilde{y}d\tilde{\xi}\, & e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\xi}}\tilde{\xi}_j\tilde{\xi}_k \\
&\times\Big[\int_0^1 d\tau_1(1-\tau_1)\partial^2_{\xi_j\xi_k} H\Big(x+\frac{\tilde{y}}{2}, \tau_1\tilde{\xi}+\widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big)\Big]\, a(x+\tilde{y},\eta).
\end{aligned}$$

As the coefficient of $|\xi|^2$ of H is constant in x, we have, for any $\tau_1 \in (0,1)$, $\tilde{\xi} \in \mathbb{R}^m$,

$$\partial^2_{\xi_j\xi_k} H\Big(x+\frac{\tilde{y}}{2}, \tau_1\tilde{\xi}+\widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big) = \partial^2_{\xi_j\xi_k} H\Big(x+\frac{\tilde{y}}{2}, \widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big). \tag{3.14}$$

Using integration by parts and applying (1.11), we have readily

(3.15)
$$\begin{aligned}
r_L(x,\eta) &= \frac{\hbar}{2i}c_m^2 \int d\tilde{y}d\tilde{\xi}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\xi}}\Big[\tilde{\xi}_k\,\partial^2_{\xi_k\xi_j} H\Big(x+\frac{\tilde{y}}{2}, \widetilde{\partial_x\phi}(x,\tilde{y},\eta)\Big)\,\partial_{x_j}a(x+\tilde{y},\eta)\Big] \\
&= -\frac{\hbar^2}{2}\partial^2_{\xi_k\xi_j}H(x,\partial_x\phi(x,\eta))\,\partial^2_{x_jx_k}a(x,\eta).
\end{aligned}$$

(II) To make the above procedure rigorous, we need to justify the usages of the changing the order of integration and those of delta functions. But, these are readily justified by using oscillatory integrals and therefore omitted here. □

REMARKS. (i) The main term is easily obtained from

$$\sum_{|\alpha|=0}^{1} \frac{(-i\hbar)^{|\alpha|}}{\alpha!} \partial_{\tilde{y}}^{\alpha} \Big(\partial_{\tilde{\xi}}^{\alpha} H(x+\frac{\tilde{y}}{2}, \tilde{\xi}+\widetilde{\partial_x \phi}(x,\tilde{y},\eta)) \cdot a(x+\tilde{y},\eta) \Big)\Big|_{\substack{\tilde{y}=0,\\ \tilde{\xi}=0}}. \tag{3.16}$$

(ii) The term $-2^{-1}i\hbar\partial^2_{x_j\xi_j}H\cdot a$ in (3.3) will not appear if we use $\hat{H}(x,D^\hbar_x)$ instead of $\hat{H}^W(x,D^\hbar_x)$.
(iii) Above arguments are applicable for more general symbol $P(x,\xi)$ satisfying, for any $j,k,\ell=1,\cdots,m$ and x,ξ,

$$\partial^3_{\xi_k x_j \xi_j} P(x,\xi)=0 \text{ and } \partial^3_{\xi_\ell \xi_k \xi_j} P(x,\xi)=0. \tag{3.17}$$

3.2. Composition of FIO with ΨDO from the right

Theorem 3.2. *Let $F(a,\phi)$, $\hat{H}^W(x,D^\hbar_x)$ be FIO and Weyl type pseudo-differential, respectively. We assume that a,ϕ as above and $H(x,\xi)$ is given by (1.16). Then, there exists $c_R=c_R(x,\xi)\in C^\infty(\mathbb{R}^{2m})$ satisfying*

$$F(a,\phi)\hat{H}^W(x,D^\hbar_x)=F(c_R,\phi). \tag{3.18}$$

with the following expansion:

$$c_R = aH - i\hbar\Big\{\partial_{\xi_j}a\cdot\partial_{x_j}H+\frac{1}{2}a\Big(\partial^2_{\xi_j x_j}H+\partial^2_{\xi_j\xi_k}\phi\cdot\partial^2_{x_k x_j}H\Big)\Big\}+r_R. \tag{3.19}$$

Here arguments of c_R, a and ϕ are (x,ξ) and that of H is $(\partial_\xi\phi(x,\xi),\xi)$, and $r_R(x,\xi)$ is expressed as

$$r_R(x,\xi)=r^{(1)}_{Ri}(x,\xi)\xi_i+r^{(0)}_R(x,\xi). \tag{3.20}$$

Proof. As before, it is enough to calculate formally which yields (3.19).
(i) By (1.20), putting

$$H^\hbar(x,\xi)=H(x,\xi)-\frac{\hbar}{2i}G(x),\quad G(x)=\frac{\partial A_i(x)}{\partial x_i}=\frac{\partial^2 H(x,\xi)}{\partial x_i\partial\xi_i},$$

we have

$$F(a,\phi)\hat{H}^W(x,D^\hbar_x)u(x)=c_m\int d\xi\, c_R(x,\xi)e^{i\hbar^{-1}\phi(x,\xi)}\hat{u}(\xi). \tag{3.21}$$

Here, we set

$$c_R(x,\xi) = c_m^2 \int dy d\eta\, e^{i\hbar^{-1}(\phi(x,\eta)-\phi(x,\xi)-y\cdot(\eta-\xi))} a(x,\eta) H^\hbar(y,\xi). \tag{3.22}$$

Using

$$\phi(x,\eta) - \phi(x,\xi) = \widetilde{\partial_{\xi_j}\phi}(x,\xi,\eta-\xi)(\eta_j - \xi_j) = \widetilde{\partial_\xi\phi}(x,\xi,\eta-\xi)\cdot(\eta-\xi),$$

where

$$\widetilde{\partial_{\xi_j}\phi}(x,\xi,\zeta) = \int_0^1 d\tau \partial_{\xi_j}\phi(x,\xi+\tau\zeta), \tag{3.23}$$

we define a change of variables as

$$\begin{cases} \tilde{y} = y - \widetilde{\partial_\xi\phi}(x,\xi,\eta-\xi), \\ \tilde{\eta} = \eta - \xi, \end{cases} \longleftrightarrow \begin{cases} y = \tilde{y} + \widetilde{\partial_\xi\phi}(x,\xi,\tilde{\eta}), \\ \eta = \tilde{\eta} + \xi. \end{cases} \tag{3.24}$$

Then, we get

$$c_R(x,\xi) = c_m^2 \int d\tilde{y} d\tilde{\eta}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}} a(x,\tilde{\eta}+\xi)\, H^\hbar(\tilde{y} + \widetilde{\partial_\xi\phi}(x,\xi,\tilde{\eta}),\xi). \tag{3.25}$$

(ii) Using Taylor's expansion for $H^\hbar(\cdots)$ w.r.t. $\tilde{y}$, we decompose

$$\begin{aligned} H^\hbar(\tilde{y} + \widetilde{\partial_\xi\phi}(x,\xi,\tilde{\eta}),\xi) &= H^\hbar(\widetilde{\partial_\xi\phi}(x,\xi,\tilde{\eta}),\xi) \\ &\quad + \tilde{y}_j \partial_{x_j} H^\hbar(\widetilde{\partial_\xi\phi}(x,\xi,\tilde{\eta}),\xi) + \tilde{y}_j\tilde{y}_k \widetilde{H^\hbar_{(kj)}}(x,\xi,\tilde{y},\tilde{\eta}) \end{aligned}$$

with

$$\widetilde{H^\hbar_{(\alpha)}}(x,\xi,\tilde{y},\tilde{\eta}) = \int_0^1 d\tau_1 (1-\tau_1)\partial_x^\alpha H^\hbar(\tau_1\tilde{y} + \widetilde{\partial_\xi\phi}(x,\xi,\tilde{\eta}),\xi).$$

So, we put

$$c_R(x,\xi) = I_1 + I_2 + I_3,$$

where

$$I_1 = c_m^2 \int d\tilde{y} d\tilde{\eta}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}}\, a(x,\tilde{\eta}+\xi)\, H^\hbar(\widetilde{\partial_\xi\phi}(x,\xi,\tilde{\eta}),\xi), \tag{3.26}$$

$$(3.27)\qquad I_2 = c_m^2 \int d\tilde{y}d\tilde{\eta}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}}\, a(x,\tilde{\eta}+\xi)\tilde{y}_j\partial_{x_j}H^\hbar(\widetilde{\partial_\xi\phi}(x,\xi,\tilde{\eta}),\xi),$$

and

$$(3.28)\qquad I_3 = c_m^2 \int d\tilde{y}d\tilde{\eta}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}} a(x,\tilde{\eta}+\xi)\tilde{y}_j\tilde{y}_k\widetilde{H^\hbar_{(kj)}}(x,\xi,\tilde{y},\tilde{\eta}).$$

(iii) Using (1.11), we get readily

$$(3.29)\qquad I_1 = a(x,\xi)H^\hbar(\partial_\xi\phi(x,\xi),\xi).$$

Remarking $\partial_{\tilde{\eta}_j} e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}} = -i\hbar^{-1}\tilde{y}_j e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}}$, integration by parts and applying (1.11), we get

(3.30)
$$I_2 = -i\hbar\Big[a_{\xi_j}(x,\xi)H^\hbar_{x_j}(\phi_\xi(x,\xi),\xi) + \frac{1}{2}a(x,\xi)\,\phi_{\xi_j\xi_\ell}(x,\xi)\,H^\hbar_{x_\ell x_j}(\phi_\xi(x,\xi),\xi)\Big].$$

Therefore, we have,

(3.31)
$$\begin{aligned} I_1 + I_2 = a\,H - i\hbar\{a_{\xi_j}H_{x_j} + \frac{1}{2}a\,(H_{x_\ell\xi_\ell} + \phi_{\xi_j\xi_\ell}\,H_{x_\ell x_j})\} \\ - \frac{\hbar^2}{2}\big[a_{\xi_j}H_{x_jx_\ell\xi_\ell} + \frac{1}{2}a\,\phi_{\xi_j\xi_\ell}\,H_{x_\ell x_jx_n\xi_n}\big], \end{aligned}$$

with arguments of a_*, ϕ_* are (x,ξ) and those of H_* are $(\partial_\xi\phi(x,\xi),\xi)$, respectively. From this, the main terms of (3.19) by picking terms of order up to 1 w.r.t. $\hbar$ from I_1+I_2.

(iv) By integration by parts, we get

$$(3.32)\qquad I_3 = -\hbar^2 c_m^2 \int d\tilde{y}d\tilde{\eta}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}}\partial^2_{\tilde{\eta}_j\tilde{\eta}_k}\big[a(x,\tilde{\eta}+\xi)\,\widetilde{H^\hbar_{(kj)}}(x,\xi,\tilde{y},\tilde{\eta})\big].$$

Therefore, we get

$$\partial^2_{\tilde{\eta}_j\tilde{\eta}_k}\big[a\cdot\widetilde{H^\hbar_{(kj)}}\big] = a_{\xi_j\xi_k}\widetilde{H^\hbar_{(kj)}} + 2a_{\xi_j}\widetilde{\phi^{(k\ell)}}\widetilde{H^\hbar_{(\ell kj)}} + a\big[\widetilde{\phi^{(jk\ell)}}\widetilde{H^\hbar_{(\ell kj)}} + \widetilde{\phi^{(k\ell)}}\widetilde{\phi^{(jn)}}\widetilde{H^\hbar_{(n\ell kj)}}\big]$$

where

$$\widetilde{\phi^{(\beta)}}(x,\xi,\tilde{\eta}) = \int_0^1 d\tau\,\tau^{|\beta|-1}\partial_\xi^\beta\phi(x,\xi+\tau\tilde{\eta})$$

and arguments of a_*, $\widetilde{H^\hbar_*}$ and $\widetilde{\phi^*}$ are $(x, \tilde\eta + \xi)$, $(x, \xi, \tilde y, \tilde\eta)$ and $(x, \xi, \tilde\eta)$, respectively.

Putting, for any F,

$$\widetilde{F_{(\alpha)}}(x,\xi,\tilde y,\tilde\eta) = \int_0^1 d\tau_1 (1-\tau_1)\partial_x^\alpha F(\tau_1 \tilde y + \widetilde{\partial_\xi \phi}(x,\xi,\tilde\eta)),$$

we have

$$\widetilde{H^\hbar_{(kj)}} = \widetilde{A_{i,(kj)}}\xi_i + \widetilde{W_{(kj)}} - \frac{\hbar}{i}\widetilde{G_{(kj)}} \text{ with } W(x) = \frac{1}{2}A_i(x)A_i(x) + V(x).$$

Therefore, we have

$$I_3 = r^{(1)}_{Ri}(x,\xi)\xi_i + \tilde r^{(0)}_R(x,\xi).$$

Here

(3.33)
$$r^{(1)}_{Ri}(x,\xi) = -\hbar^2 c_m^2 \int d\tilde y d\tilde\eta\, e^{-i\hbar^{-1}\tilde y\cdot\tilde\eta}\big[a_{\xi_j\xi_k}\widetilde{A_{i(kj)}} + 2a_{\xi_j}\widetilde{\phi^{(k\ell)}}\widetilde{A_{i(\ell kj)}} + a\big(\widetilde{\phi^{(jk\ell)}}\widetilde{A_{i(\ell kj)}} + \widetilde{\phi^{(k\ell)}}\widetilde{\phi^{(jn)}}\widetilde{A_{i(n\ell kj)}}\big)\big],$$

(3.34)
$$\begin{aligned}\tilde r^{(0)}_R(x,\xi) = &-\hbar^2 c_m^2 \int d\tilde y d\tilde\eta\, e^{-i\hbar^{-1}\tilde y\cdot\tilde\eta}[a_{\xi_j\xi_k}\widetilde{W_{(kj)}} + 2a_{\xi_j}\widetilde{\phi^{(k\ell)}}\widetilde{W_{(\ell kj)}} \\ &\qquad + a(\widetilde{\phi^{(jk\ell)}}\widetilde{W_{(\ell kj)}} + \widetilde{\phi^{(k\ell)}}\widetilde{\phi^{(jn)}}\widetilde{W_{(n\ell kj)}})] \\ &+ i\frac{\hbar^3}{2}c_m^2 \int d\tilde y d\tilde\eta\, e^{-i\hbar^{-1}\tilde y\cdot\tilde\eta}[a_{\xi_j\xi_k}\widetilde{G_{(kj)}} + 2a_{\xi_j}\widetilde{\phi^{(k\ell)}}\widetilde{G_{(\ell kj)}} \\ &\qquad + a(\widetilde{\phi^{(jk\ell)}}\widetilde{G_{(\ell kj)}} + \widetilde{\phi^{(k\ell)}}\widetilde{\phi^{(jn)}}\widetilde{G_{(n\ell kj)}})],\end{aligned}$$

where arguments of a_*, $\widetilde{A_*}$ and $\widetilde{\phi^*}$ are $(x, \tilde\eta+\xi)$, $(x,\xi,\tilde y,\tilde\eta)$ and $(x,\xi,\tilde\eta)$, respectively.

Finally, we put

(3.35)
$$r^{(0)}_R(x,\xi) = -\frac{\hbar^2}{2}\big[a_{\xi_j}H_{x_j x_\ell \xi_\ell} + \frac{1}{2}a\,\partial_{\xi_j\xi_\ell}\phi\, H_{x_\ell x_j x_n \xi_n}\big] + \tilde r^{(0)}_R(x,\xi),$$

where arguments of a_* and ϕ_* are (x,ξ) and those of H_* are $(\partial_\xi\phi(x,\xi),\xi)$, in other lines, arguments of integrand functions are the same as before. □

REMARKS. (i) The main term of expansion of c_R is given by

$$\sum_{|\alpha+\beta|=0}^{1} \frac{(-i\hbar)^\alpha}{\alpha!}\frac{(i\hbar)^\beta}{\beta!}\partial_{\tilde{\xi}}^{\alpha}\partial_{\tilde{\eta}}^{\beta}\Big(a(x,\tilde{\xi}+\xi)\cdot\partial_{\tilde{z}}^{\alpha}\partial_{\tilde{y}}^{\beta}H\Big(\frac{\tilde{y}}{2}+\tilde{z}+\widetilde{\partial_\xi\phi}(x,\tilde{\xi},\xi), \tilde{\eta}+\tilde{\xi}+\xi\Big)\Big)\Big|_{\substack{\tilde{y}=\tilde{z}=0,\\ \tilde{\xi}=\tilde{\eta}=0}}. \tag{3.36}$$

In fact, this formula is obtained for any ΨDO P as follows:
Using $u(z)=c_m\int d\xi' e^{i\hbar^{-1}z\cdot\xi'}\hat{u}(\xi')$, we have

(3.37)
$$\begin{aligned} F(a,\phi)\hat{P}^W(x,D_x^\hbar)u(x) &= c_m^4\int d\xi dy d\eta dz\, e^{i\hbar^{-1}(\phi(x,\xi)-y\cdot\xi+(y-z)\cdot\eta)}a(x,\xi)P\Big(\frac{y+z}{2},\eta\Big)u(z)\\ &= c_m\int d\xi'\, e^{i\hbar^{-1}\phi(x,\xi')}c_R(x,\xi')\hat{u}(\xi'). \end{aligned}$$

Here, we set

$$c_R(x,\xi')=c_m^4\int d\xi dy d\eta dz\, e^{i\hbar^{-1}\psi(x,\xi,y,\eta,z,\xi')}q(x,\xi,y,\eta,z) \tag{3.38}$$

with

$$\psi(x,\xi,y,\eta,z,\xi')=-y\cdot\xi+(y-z)\cdot\eta+z\cdot\xi'+\phi(x,\xi)-\phi(x,\xi'),$$

$$q(x,\xi,y,\eta,z)=a(x,\xi)P\Big(\frac{y+z}{2},\eta\Big).$$

Using (3.23) and

$$\phi(x,\xi)-\phi(x,\xi')=\widetilde{\partial_{\xi_j'}\phi}(x,\xi',\xi-\xi')(\xi_j-\xi_j')=\widetilde{\partial_{\xi'}\phi}(x,\xi',\xi-\xi')\cdot(\xi-\xi'),$$

where

$$\widetilde{\partial_{\xi_j'}\phi}(x,\xi',\zeta)=\int_0^1 d\tau\partial_{\xi_j'}\phi(x,\xi'+\tau\zeta),$$

we define a change of variables as

$$\begin{cases}\tilde{\xi}=\xi-\xi',\\ \tilde{y}=y-z,\\ \tilde{z}=z-\widetilde{\partial_{\xi'}\phi}(x,\xi',\xi-\xi'),\\ \tilde{\eta}=\eta-\xi,\end{cases}\longleftrightarrow\begin{cases}\xi=\xi'+\tilde{\xi},\\ y=\tilde{y}+\tilde{z}+\widetilde{\partial_{\xi'}\phi}(x,\xi',\tilde{\xi}),\\ z=\tilde{z}+\widetilde{\partial_{\xi'}\phi}(x,\xi',\tilde{\xi}),\\ \eta=\tilde{\eta}+\tilde{\xi}+\xi'.\end{cases} \tag{3.39}$$

Rewriting

$$\psi(x,\xi,y,\eta,z,\xi') = (y-z)\cdot(\eta-\xi) + (z-\widetilde{\partial_{\xi'}\phi})\cdot(\xi'-\xi),$$

we get

(3.40)

$$c_R(x,\xi') = c_m^4 \int d\tilde{\xi}d\tilde{y}d\tilde{\eta}d\tilde{z}\, e^{i\hbar^{-1}(\tilde{y}\cdot\tilde{\eta}-\tilde{z}\cdot\tilde{\xi})} a(x,\tilde{\xi}+\xi')P\Big(\frac{\tilde{y}}{2}+\tilde{z}+\widetilde{\partial_{\xi'}\phi}(x,\xi,\xi'),\tilde{\eta}+\tilde{\xi}+\xi'\Big).$$

Applying Taylor's expansion for $P(\cdots)$ w.r.t. $\frac{\tilde{y}}{2}+\tilde{z}$, we have (3.36) as the first and second terms.
(ii) If the so-called Coulomb gauge $G(x) = 0$ is imposed, then the expression of the remainder term in (3.31) and (3.34) is considerably simplified.

4. Definition and properties of parametrix

4.1. Definition of parametrix

Using functions $S(t,s,x,\xi)$ and $\mu(t,s,x,\xi) = \mathcal{D}^{1/2}(t,s,x,\xi)$ defined in §2, we consider an integral transformation $E(t,s)$ on $\mathcal{S}(\mathbb{R}^m)$:

(4.1)

$$\begin{aligned} E(t,s)u(x) = E(t,s:\mu,S)u(x) &= c_m \int_{\mathbb{R}^m} d\xi\, \mu(t,s,x,\xi)e^{i\hbar^{-1}S(t,s,x,\xi)}\hat{u}(\xi) \\ &= c_m^2 \int_{\mathbb{R}^{2m}} d\xi dy\, \mu(t,s,x,\xi)e^{i\hbar^{-1}(S(t,s,x,\xi)-y\cdot\xi)}u(y). \end{aligned}$$

Lemma 4.1. *Assume* (A), (V) *and* $|t-s| \le \delta_1$ *(defined in Proposition 2.3). Then, for any* $\hat{u} \in C_0^\infty(\mathbb{R}^m)$*, there exists a constant C such that*

$$\|E(t,s)u\| \le C\|u\|. \tag{4.2}$$

Proof. Since we have (2.31) and (2.45), we may apply Proposition 1.8. □

Proposition 4.2. (1) *For each* $u \in L^2(\mathbb{R}^m)$*, we have*

$$\operatorname*{s-lim}_{|t-s|\to 0} E(t,s)u = u \quad in \quad L^2(\mathbb{R}^m). \tag{4.3}$$

(2) *If we set* $E(s,s) = I$*, then the correspondence* $(s,t) \to E(t,s)u$ *gives a strongly continuous function with values in* $L^2(\mathbb{R}^m)$.

Proof. See Lemma 4.2 of [11]. □

4.2. Approximate estimate

Proposition 4.3. *Let $u \in \mathcal{S}(\mathbb{R}^m)$. For any fixed $x \in \mathbb{R}^m$, $E(t,s)u(x)$ is absolutely continuous in t, and its derivative is represented as*

$$\frac{\partial}{\partial t}E(t,s)u(x) = c_m \int d\xi \, \frac{\partial}{\partial t}\left[\mu(t,s,x,\xi)e^{i\hbar^{-1}S(t,s,x,\xi)}\right]\hat{u}(\xi). \tag{4.4}$$

Moreover, for any $x \in \mathbb{R}^m$, we have

$$\frac{\hbar}{i}\frac{\partial}{\partial t}E(t,s)u(x) = -\hat{H}^W(t,x,D_x^\hbar)E(t,s)u(x) + G_L(t,s)u(x). \tag{4.5}$$

Here, $G_L(t,s)$ satisfies

$$\|G_L(t,s)u\| \le C\hbar^2|t-s|\|u\|, \tag{4.6}$$

where C is independent of t, s, u and $\hbar$, $0 < \hbar \le 1$.

Proof. (4.4) follows directly from the definition of the oscillatory integral and Lebesgue's dominated convergence theorem. Using the Hamilton-Jacobi and the continuity equations with the product formula in Theorem 3.1, we get

$$\begin{aligned}\frac{\hbar}{i}(\mu_t + i\hbar^{-1}S_t\,\mu) &= i\hbar\left[\mu_{x_j}H_{\xi_j} + (1/2)(H_{x_j\xi_j} + H_{\xi_j\xi_k}S_{x_jx_k})\mu\right] - \mu H \\ &= -[\text{amplitude part of the "symbol" of } (\hat{H}^W(t,x,D_x)E(t,s))] + r_L.\end{aligned} \tag{4.7}$$

Here, arguments of r_L, μ and S are (t,s,x,ξ) and those of H are $(x, \partial_x S(t,s,x,\xi))$. Moreover, as $r_L = r_L(t,s,x,\xi) = -\frac{\hbar^2}{2}\Delta_x\mu(t,s,x,\xi)$ by (3.4), it has the following estimate: for any multi-indeces α and β, there exists a positive constant $C_{\alpha,\beta}$ such that

$$|\partial_x^\alpha\partial_\xi^\beta r_L(t,s,x,\xi)| \le C_{\alpha\beta}\hbar^2|t-s|. \tag{4.8}$$

Therefore, putting

$$G_L(t,s)u(x) = c_m \int d\xi \, r_L(t,s,x,\xi)e^{i\hbar^{-1}S(t,s,x,\xi)}\hat{u}(\xi),$$

we get (4.6) by (4.8). □

REMARK. One of the main reason why we use μ instead of 1 as the amplitude of $E(t,s)$, is to have the equality (4.7). More essentially, see Inoue-Maeda [9] for the introduction of the intrinsic Hilbert space. Analogously as above, we have

Proposition 4.4. *Let $u \in \mathcal{S}(\mathbb{R}^m)$. For any fixed $x \in \mathbb{R}^m$, $E(t,s)u(x)$ is absolutely continuous in s, and its derivatives are represented as*

$$\frac{\partial}{\partial s}E(t,s)u(x) = c_m \int d\xi \, \frac{\partial}{\partial s}[\mu(t,s,x,\xi)e^{i\hbar^{-1}S(t,s,x,\xi)}]\hat{u}(\xi). \tag{4.9}$$

Moreover, for any $x \in \mathbb{R}^m$, we have

$$\frac{\hbar}{i}\frac{\partial}{\partial s}E(t,s)u(x) = E(t,s)\hat{H}^W(s,x,D_x)u(x) + G_R(t,s)u(x). \tag{4.10}$$

Here, $G_R(t,s)$ have the following estimates.

$$\|G_R(t,s)u\| \le C\hbar^2|t-s| \, |||u|||_1 \tag{4.11}$$

where C is independent of t, s, u and $\hbar$, $0 < \hbar \le 1$.

Proof. We claim that for any α, β, we have

$$|\partial_x^\alpha \partial_\xi^\beta r_{Ri}^{(1)}(t,s,x,\xi)| \le C_{\alpha\beta}\hbar^2|t-s|,$$
$$|\partial_x^\alpha \partial_\xi^\beta r_R^{(0)}(t,s,x,\xi)| \le C_{\alpha\beta}\hbar^2|t-s|,$$

where $r_{Ri}^{(1)}(t,s,x,\xi)$ and $r_R^{(0)}(t,s,x,\xi)$ are defined in (3.33) and (3.34). As other terms are analogously estimated, we only prove the first term in (3.33) satisfies the claim: Thus putting

$$b_i(t,s,x,\xi) = -\hbar^2 c_m^2 \int d\tilde{y}d\tilde{\eta}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}}\mu_{\xi_j\xi_k}(t,s,x,\xi+\tilde{\eta})\widetilde{A_{i(kj)}}(s,x,\xi,\tilde{y},\tilde{\eta}),$$

we may claim

$$|\partial_x^\alpha \partial_\xi^\beta b_i(t,s,x,\xi)| \le C_{\alpha\beta}\hbar^2|t-s|.$$

This follows from the definition of oscillatory integrals appearing in Proposition 1.2, see, for example, [13] and [12]. In fact, taking $2\ell, 2\ell' > m$, we have

$$\begin{aligned}
&\int d\tilde{y}d\tilde{\eta}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}}\mu_{\xi_j\xi_k}(t,s,x,\xi+\tilde{\eta})\widetilde{A_{i(kj)}}(s,x,\xi,\tilde{y},\tilde{\eta}) \\
&\quad = \int d\tilde{y}d\tilde{\eta}\, e^{-i\hbar^{-1}\tilde{y}\cdot\tilde{\eta}}\langle\tilde{\eta}\rangle^{-2\ell}\langle D_{\tilde{y}}^{\hbar}\rangle^{-2\ell}\langle\tilde{y}\rangle^{-2\ell'}\langle D_{\tilde{\eta}}^{\hbar}\rangle^{-2\ell'}\mu_{\xi_j\xi_k}(t,s,x,\xi+\tilde{\eta}) \\
&\qquad\qquad \times \widetilde{A_{i(kj)}}(s,x,\xi,\tilde{y},\tilde{\eta}) \\
&\quad = \int d\tilde{y}d\tilde{\eta}\, [\langle\tilde{\eta}\rangle^{-2\ell}\langle\tilde{y}\rangle^{-2\ell'}\{\text{bounded functions}\} + \textit{etc.}]. \qquad \square
\end{aligned}$$

Corollary 4.5. *In case $A_i(t,x) = a_{ij}(t)x_j$, we have*

$$\|G_R(t,s)u\| \le C\hbar^2|t-s|\|u\|. \tag{4.12}$$

Proof. In this case, as $\widetilde{A_{i(\alpha)}} = 0, |\alpha| \ge 2$, we have $r_{Ri}^{(1)} = 0$. □

Proposition 4.6. *There exists a positive constant C such that for $u \in \mathcal{S}(\mathbb{R}^m)$,*

$$\|(E(t,s_1)E(s_1,s) - E(t,s))u\| \le C\hbar(|t-s_1|^2 + |s_1-s|^2)|||u|||_1, \tag{4.13}$$

$$\|(E(s_1,t)^*E(s_1,s) - E(t,s))u\| \le C\hbar(|t-s_1|^2 + |s_1-s|^2)\|u\|. \tag{4.14}$$

Proof. Let $u \in \mathcal{S}(\mathbb{R}^m)$. Then, we have by Propositions 4.3 and 4.4,

$$\begin{aligned}\|\frac{d}{d\sigma}E(t,\sigma)E(\sigma,s)u\| &= \|i\hbar^{-1}G_R(t,\sigma)E(\sigma,s)u + i\hbar^{-1}E(t,\sigma)G_L(\sigma,s)u\| \\ &\le C\hbar(|t-\sigma| + |\sigma-s|)|||u|||_1.\end{aligned} \tag{4.15}$$

After integrating with respect to σ from s to s_1, we get (4.13). On the other hand, remarking

$$(E(s_1,s)u, E(s_1,t)w) - (E(t,s)u,w) = -\frac{d}{d\tau}(E(\tau,s)u, E(\tau,t)w)\Big|_{\tau=s_1}^{\tau=t},$$

we get (4.14). □

As a corollary of (4.14), we get

Corollary 4.7.

$$\|E(t,s)\| \le e^{C\hbar|t-s|^2}. \tag{4.16}$$

4.3. Regularity

Fix $T > 0$ arbitrary, and assume $t, s, s_1 \in [-T,T]$ such that $t, s_1 \in [s-\delta_1/2, s+\delta_1/2]$, where δ_1 is defined in Proposition 2.3.

Lemma 4.8. (Proposition 6.1 of [11]) *Let $|t-s| < \delta_1$ and $u \in \mathcal{S}(\mathbb{R}^m)$. Then, we have the following:*
(1) *For any multi-indices α, β and j $(1 \le j \le m)$,*

$$\begin{cases} \|x^\alpha\partial_x^\beta[\partial_{x_j}, E(t,s)]u\| \le C_{\alpha\beta}|t-s| \; |||u|||_{|\alpha|+|\beta|+1}, \\ \|x^\alpha[x_j, E(t,s)]u\| \le C_\alpha|t-s| \; |||u|||_{|\alpha|+1} \end{cases} \tag{4.17}$$

where constants $C_{\alpha\beta}$ and C_α are independent of t, s and u.
(2) *Moreover, we have, for any α, β,*

$$\|x^\alpha \partial_x^\beta E(t,s)u\| \le e^{C|t-s|}\|x^\alpha \partial_x^\beta u\| + C_{\alpha\beta}|t-s| \; |||u|||_{|\alpha|+|\beta|} \tag{4.18}$$

for some constants C and $C_{\alpha\beta}$ independent of t, s and u.
(3) *For $k \in \mathbf{Z}_+$, we have*

$$|||E(t,s)u|||_k \le e^{C|t-s|}|||u|||_k \tag{4.19}$$

with some constant $C > 0$. This implies that $E(t,s)u \in \mathcal{S}(\mathbb{R}^m)$ for $u \in C_0^\infty(\mathbb{R}^m)$.

Proof. (4.19) follows from (4.17). Using (4.19) and the Sobolev imbedding theorem, we get the last assertion. In fact, we get for any ℓ, α, there exist constants C, C' and k such that

$$|\langle x\rangle^\ell \partial_x^\alpha E(t,s)u(x)| \le C|||E(t,s)u|||_k \le C'|||u|||_k. \tag{4.20}$$

□

5. Composition of FIOs

In order to apply diectly the theorem of Fujiwara or Kitada, the estimate (4.13) is insufficient. We calculate the quantity $\|E(t,s)E(s,r)u - E(t,r)u\|$ directly.

Lemma 5.1. *Let $|t-s| + |s-r|$ be sufficiently small. For any x, ξ, there exists a unique solution (X, Ξ), $X = X(t,s,r,x,\xi)$, $\Xi = \Xi(t,s,r,x,\xi)$ of*

$$\begin{cases} X_j = \partial_{\xi_j} S(t,s,x,\Xi), \\ \Xi_j = \partial_{x_j} S(s,r,X,\xi). \end{cases} \tag{5.1}$$

Moreover, we have

$$\begin{aligned} |\partial_x^\alpha \partial_\xi^\beta (X_j - x_j)| &\le C_{\alpha,\beta}(1+|x|+|\xi|)^{(1-|\alpha+\beta|)_+}, \\ |\partial_x^\alpha \partial_\xi^\beta (\Xi_j - \xi_j)| &\le C_{\alpha,\beta}(1+|x|+|\xi|)^{(1-|\alpha+\beta|)_+}. \end{aligned} \tag{5.2}$$

Proof. See, Kumano-go, Taniguchi & Tozaki [15], Propositions 2.2 and 2.4 of [12]. □

Putting

$$\Phi(t,s,r,x,\xi) = S(t,s,x,\Xi) - X\Xi + S(s,r,X,\xi),$$

we have,

Lemma 5.2.

$$
(5.3)\qquad \begin{cases} \dfrac{\partial}{\partial s}\Phi(t,s,r,x,\xi)=0, \\ \dfrac{\partial}{\partial t}\Phi(t,s,r,x,\xi)=-H(t,x,\partial_x\Phi(t,s,r,x,\xi)), \\ \dfrac{\partial}{\partial r}\Phi(t,s,r,x,\xi)=H(r,\partial_\xi\Phi(t,s,r,x,\xi),\xi). \end{cases}
$$

Proof. The first equality is obtained by using the Hamilton-Jacobi equation and (5.1) as follows:

$$
\begin{aligned}
&\frac{\partial}{\partial s}\Phi(t,s,r,x,\xi) \\
&\quad = \partial_s S(t,s,x,\Xi) + \frac{\partial \Xi}{\partial s}\partial_\xi S(t,s,x,\Xi) - \frac{\partial X}{\partial s}\Xi - X\frac{\partial \Xi}{\partial s} \\
&\qquad + \partial_s S(s,r,X,\xi) + \frac{\partial X}{\partial s}\partial_x S(s,r,X,\xi) \\
&\quad = H(s,\partial_\xi S(t,s,x,\Xi),\Xi) - H(s,X,\partial_x S(s,r,X,\xi)) = 0.
\end{aligned}
$$

Analogously, we have other equalities. □

Corollary 5.3. *Let $|t-s|+|s-r|$ be sufficiently small. For any s satisfying this, we have*

$$
(5.4)\qquad \Phi(t,s,r,x,\xi)=S(t,r,x,\xi).
$$

Proof. In fact, by making $s\to r$,

$$
\Xi_j=\partial_{x_j}S(r,r,X,\xi)=\xi_j,\quad X_j=\partial_{\xi_j}S(t,r,x,\xi),
$$

we get

$$
\Phi(t,r,r,x,\xi)=S(t,r,x,\Xi)-X\Xi+S(r,r,X,\xi)=S(t,r,x,\xi).
$$

By the first equality in (5.3), we have

$$
0=\int_r^s ds\frac{\partial}{\partial s}\Phi(t,s,r,x,\xi)=\Phi(t,s,r,x,\xi)-\Phi(t,r,r,x,\xi). \qquad \square
$$

REMARK. $\Phi(t,s,r,x,\xi)$ is called a $\#$-product of $S(t,s,x,\xi)$ and $S(s,r,x,\xi)$, and which is denoted by $S(t,s,x,\cdot)\#S(s,r,\cdot,\xi)$ in [15]. Now, we have, as an oscillatory integral,

$$
\begin{aligned}
&E(t,s)E(s,r)u(x) = \\
(5.5)\qquad &c_m^3 \int_{\mathbb{R}^{3m}} d\eta\, dy\, d\xi\, \mu(t,s,x,\eta)\mu(s,r,y,\xi) e^{i\hbar^{-1}(S(t,s,x,\eta)-y\eta+S(s,r,y,\xi))}\,\hat{u}(\xi).
\end{aligned}
$$

Using the change of variables

$$
y = X + \tilde{y}, \quad \eta = \Xi + \tilde{\eta},
$$

and (5.4), we have

$$
(5.6)\qquad S(t,s,x,\eta) - y\eta + S(s,r,y,\xi) - S(t,r,x,\xi) = -\tilde{y}\tilde{\eta} + R(t,s,r,x,\xi,\tilde{y},\tilde{\eta})
$$

with

$$
\begin{aligned}
&R(t,s,r,x,\xi,\tilde{y},\tilde{\eta}) \\
&= S(t,s,x,\Xi+\tilde{\eta}) - S(t,s,x,\Xi) - X\tilde{\eta} + S(s,r,X+\tilde{y},\xi) - S(s,r,X,\xi) - \tilde{y}\Xi \\
&= \tilde{\eta}_k\tilde{\eta}_j \int_0^1 d\tau (1-\tau) S_{\xi_j\xi_k}(t,s,x,\Xi+\tau\tilde{\eta}) + \tilde{y}_k\tilde{y}_j \int_0^1 d\tau(1-\tau) S_{x_jx_k}(s,r,X+\tau\tilde{y},\xi).
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&c_m^2 \int_{\mathbb{R}^{2m}} d\eta\, dy\, \mu(t,s,x,\eta)\mu(s,r,y,\xi) e^{i\hbar^{-1}(S(t,s,x,\eta)-y\eta+S(s,r,y,\xi))} \\
&= e^{i\hbar^{-1}S(t,r,x,\xi)} \left[c_m^2 \int_{\mathbb{R}^{2m}} d\tilde{\eta}\, d\tilde{y}\, \mu(t,s,x,\Xi+\tilde{\eta})\mu(s,r,X+\tilde{y},\xi) e^{i\hbar^{-1}(R(t,s,r,x,\xi,\tilde{y},\tilde{\eta})-\tilde{y}\tilde{\eta})} \right].
\end{aligned}
$$

Putting

$$
(5.7)\quad E(t,s)E(s,r)u(x) - E(t,r)u(x) = c_m \int_{\mathbb{R}^m} d\xi\, b(t,s,r,x,\xi) e^{i\hbar^{-1}S(t,r,x,\xi)}\,\hat{u}(\xi)
$$

with

$$
\begin{aligned}
&b(t,s,r,x,\xi) = \\
&c_m^2 \int_{\mathbb{R}^{2m}} d\tilde{\eta}\, d\tilde{y}\, \mu(t,s,x,\Xi+\tilde{\eta})\mu(s,r,X+\tilde{y},\xi) e^{i\hbar^{-1}(R(t,s,r,x,\xi,\tilde{y},\tilde{\eta})-\tilde{y}\tilde{\eta})} - \mu(t,r,x,\xi),
\end{aligned}
$$

we want to have

Proposition 5.4. *Under the assumptions (A) and (V), if $|t-s|+|s-r|$ is sufficiently small, we have*

$$|\partial_x^\alpha \partial_\xi^\beta b(t,s,r,x,\xi)| \le C_{\alpha,\beta}(|t-s|^2+|s-r|^2). \tag{5.8}$$

This estimate is conjectured in [8] and then proved by K. Taniguchi [17].
From (5.8), we have proved

Corollary 5.5. *There exists a constant C such that if $|t-s|+|s-r|\le\delta$ and $u\in\mathcal{S}(\mathbb{R}^m)$,*

$$\|E(t,s)E(s,r)u - E(t,r)u\| \le C(|t-s|^2+|s-r|^2)\|u\|. \tag{5.9}$$

6. Proof of Main Theorem

We apply the abstract theorem in Appendix A: Put

$$X_0 = X_1 = L^2(\mathbb{R}^m), \text{ with norm } \|\cdot\|_0 = \|\cdot\|_1 = \|\cdot\|,$$
$$D=\mathcal{S}(\mathbb{R}^m),\ W=Y_2,\ F(t,s)=E(t,s),\ \alpha=\gamma=2,$$
$$A_0(t)=i\hbar^{-1}\hat{H}^W(t,x,D^\hbar),\ A(t)=\text{the closed extension of } i\hbar^{-1}\hat{H}^W(t,x,D^\hbar) \text{ with domain } Y_2.$$

Then, we have that $U(t,s)=\lim_{\delta(\Delta)\to 0}E(\Delta|t,s)$ in the operator norm in $L^2(\mathbb{R}^m)$. More precisely, (A1) is given by (4.16), (A2) is proved in (5.9), and Proposition 4.2 gives (A3). Therefore, there exists a family of bounded operators $\{U(t,s)\}$ satisfying (1) and (2) of Main Theorem. Assumption (iii) of Proposition A4 is proved by remarking (4.19) (see the proof of Theorem 4 of [6]). (A6) is proved in Proposition 4.3. These imply (3) of Main Theorem. The isometry of the operators $U(t,s)$ and $U(s,t)$ are derived from the formal self-adjointness of $\mathbb{H}(t,x,D_x^\hbar)$ and the equations (3) in Main Theorem. Therefore, the operator $U(t,s)$ is unitary. □

REMARK. In case when we have only the estimate (4.13) instead of (5.9), we show the strong convergence of the Cauchy net $\{E(\Delta|t,s)u\}$. In fact, we may apply the abstract theorem by putting

$$X_0=L^2(\mathbb{R}^m),\ X_1=Y_1 \text{ with norms } \|\cdot\|_0=\|\cdot\|,\ \|\cdot\|_1=|||\cdot|||_1,$$
$$D=\mathcal{S}(\mathbb{R}^m),\ W=Y_2,\ F(t,s)=E(t,s),\ \alpha=\gamma=2,$$
$$A_0(t)=i\hbar^{-1}\hat{H}^W(t,x,D^\hbar),\ A(t)=\text{the closed extension of } i\hbar^{-1}\hat{H}^W(t,x,D^\hbar) \text{ with domain } Y_2.$$

Then, for $U\in D$, we have $U(t,s)u = s-\lim_{\delta(\Delta)\to 0}E(\Delta|t,s)u$, that is,

$$\|U(t,s)u - E(\Delta|t,s)u\|_0 \le C\delta(\Delta)^{\alpha-1}|||u|||_1.$$

A Abstract Product formula

For the self-containedness of this paper, we modify and extend slightly Fujiwara's argument (see also Theorems 2.1, 2.4 of [11], Theorems A, B of [10]).

Theorem A1. *Let X_j $(j = 0, 1)$ be two Banach spaces with norms $\|\cdot\|_0$, $\|\cdot\|_1$, respectively. X_1 is assumed to be continuously and densely imbedded in X_0. Let D be a dense subspace of each X_j $(j = 0, 1)$. Let a family of linear operators $\{F(t,s) \,|\, (t,s) \in [-T,T]^2,\ |t-s| \le 1\}$ for $T > 0$ acting on X_j, be given with the following properties:*

(1) *For each j, $F(t,s)$ is a bounded operator on X_j such that there exist a constant $C_1 > 0$ and $\gamma_j \ge 1$ satisfying*

$$\text{(A1)} \qquad \|F(t,s)u\|_j \le e^{C_1|t-s|^{\gamma_j}}\|u\|_j \ \text{for}\ j = 0, 1.$$

(2) *There exist $\alpha > 1$ and C_2 such that for any $u \in X_1$,*

$$\text{(A2)} \qquad \|(F(t,s_1)F(s_1,s) - F(t,s))u\|_0 \le C_2(|t-s_1|^\alpha + |s_1-s|^\alpha)\|u\|_1.$$

(3) *For $u \in D$, $F(t,s)u$ is a X_0-valued strongly continuous function in $(t,s) \in \mathbb{R}^2$ and it satisfies*

$$\text{(A3)} \qquad \begin{cases} F(s,s)u = u \ \text{for any}\ s \in \mathbb{R}, \\ \lim_{t\to s} \|F(t,s)u - u\|_0 = 0. \end{cases}$$

For a subdivision Δ of (s,t) such that

$$\Delta : t_0 = s < t_1 < \cdots < t_{\ell-1} < t_\ell = t \ \text{and}\ \delta(\Delta) = \max_{j=1,\cdots,\ell} |t_j - t_{j-1}|,$$

we put

$$F(\Delta|t,s)u = F(t,t_{\ell-1})F(t_{\ell-1},t_{\ell-2})\cdots F(t_1,s).$$

Then, for any $u \in D$, there exists a limit

$$\text{(A4)} \qquad U(t,s)u = \operatorname*{s-lim}_{\delta(\Delta)\to 0} F(\Delta|t,s)u \quad \text{in}\ X_0$$

such that

$$\text{(A5)} \qquad \|(U(t,s) - F(\Delta|t,s))u\|_0 \le C_3|t-s|\delta(\Delta)^{\alpha-1}\|u\|_1,$$

Here, $C_3 = C_2\big[(1-2^{1-\alpha})^{-1} + 2^{(\alpha-1)}(e(\alpha-1)\log 2)^{-1}\big]$. *We have also,*

(A6) $$\|U(t,s)u\|_j \le e^{C_1|t-s|}\|u\|_j \ \text{for}\ j=0,1.$$

Moreover, if we put $U(s,s)=I$ *for* $|s|\le T$, *then*

1. *the mapping:* $[-T,T]^2 \ni (t,s) \to U(t,s)u \in X_0$ *is continuous for any* $u \in X_0$,
2. *(evolutional property)*

$$U(t_1,t_2)U(t_2,t_3)u = U(t_1,t_3)u \ \text{ for any } \ |t_j|\le T.$$

For the proof, we prepare the following lemmas:

Lemma A2. *Let* $\Delta_L = \{t_j\}$ *with* $t_j = s + jL^{-1}(t-s)$ *for* $j = 0,1,\cdots,L$ *and* $\delta(\Delta_L) = L^{-1}|t-s|$. *We have*

(A7) $$\|(F(t,s)-F(\Delta|t,s))u\|_0 \le C_3|t-s|^\alpha e^{C_1|t-s|}\|u\|_1,$$

where $F(\Delta_L|t,s)u = F(t_L,t_{L-1})\cdots F(t_1,t_0)u$.

Proof of this lemma is obtained from Lemma 5.7 of [6].

Lemma A3. *Let two subdivisions of* $[s,t]$ *be given by*

$$\Delta_1 : s = t_0 < t_1 < \cdots < t_{L-1} < t_L = t$$

$$\Delta_2 : s = s_0 < s_1 < \cdots < s_{M-1} < s_M = t.$$

Assuming that $\delta(\Delta_1) < \delta_1$ *and* $\delta(\Delta_2) < \delta_1$, *we get*

(A8)
$$\|(F(\Delta_1|t,s)-F(\Delta_2|t,s))u\|_0 \le C_3|t-s|(\delta(\Delta_1)^{\alpha-1}+\delta(\Delta_2)^{\alpha-1})e^{C_1|t-s|}\|u\|_1.$$

This lemma corresponds to Lemma 5.8 of [6], therefore the proof is omitted.

Proof of Theorem. A1 By the above lemma, we get (A4). Moreover, as is proved in Theorem 4 of [6], we have the estimates (A6).

Concerning the evolutional property for $s<r<t$, we take the subdivision Δ containing r, i.e.

$$\Delta = \Delta_l \cup \Delta_r \ \text{ with } \ \Delta_l : s = t_0 < t_1 < \cdots < t_L = r < t_{L+1}, \quad \Delta_r : t_L = r < t_{L+1} < \cdots < t_M = t.$$

Then, remarking $F(\Delta_r|t,r)F(\Delta_l|r,s) = F(\Delta|t,s)$, we get

$$\begin{aligned}\|U(t,r)U(r,s)u - U(t,s)u\|_0 &\le \|((U(t,r) - F(\Delta_r|t,r))U(r,s)u\|_0 \\ &+ \|F(\Delta_r|t,r)(U(r,s) - F(\Delta_l|r,s))u\|_0 \\ &+ \|(F(\Delta_r|t,r)F(\Delta_l|r,s) - U(t,s))u\|_0 \to 0 \quad \text{when } \delta(\Delta) \to 0.\end{aligned}$$

In fact, for $u \in D$, we have

$$\begin{aligned}&\|((U(t,r) - F(\Delta_r|t,r))U(r,s)u\|_0 \le C|t-r|\delta(\Delta_r)^{\alpha-1}\|U(r,s)u\|_1 \\ &\le C|t-r|\delta(\Delta_r)^{\alpha-1}e^{C_1|r-s|}\|u\|_1 \to 0 \quad \text{when } \delta(\Delta) \to 0.\end{aligned}$$

□

Proposition A4. *Under the same assumption as above, we assume that:*
(i) *There exist a closed operator $A(t)$ with domain $D(A(t))$ in X_0.*
(ii) *For $u \in D$, $F(t,s)u \in D(A(t))$ and $F(t,s)u$ is X_0-valued differentiable in $t \in \mathbb{R}$ and*

$$\frac{\partial}{\partial t}F(t,s)u\Big|_{s=t} + A(t)u = 0, \text{ that is, } \lim_{h\to 0}\|\frac{1}{h}(F(t+h,t) - I)u + A(t)u\|_0 = 0.$$

(iii) $\|U(t,s)u\|_j \le C\|u\|_j$ *for $u \in D$.*
Then, we have

$$\text{(A9)} \qquad \begin{cases} \dfrac{\partial}{\partial t}U(t,s)u + A(t)U(t,s)u = 0, \\ \dfrac{\partial}{\partial s}U(t,s)u - U(t,s)A(s)u = 0. \end{cases}$$

Proof. The first one is easily seen from

$$\begin{aligned}&\|\frac{1}{h}(U(t+h,s) - U(t,s))u + A(t)U(t,s)u\|_0 \\ &\le \|\frac{1}{h}(U(t+h,t) - F(t+h,t))U(t,s)u\|_0 \\ &\quad + \|\frac{1}{h}(F(t+h,t) - I)U(t,s)u + A(t)U(t,s)u\|_0 \\ &\to 0 \quad \text{as } h \to 0.\end{aligned}$$

Because, the first term is majorized by $h^{\alpha-1}\|u\|_1$ and the second term tends to 0 when $h \to 0$ by (ii) and $U(t,s)u \in Y_1$ for $u \in D$ by (iii).

The second one is given by

$$\|\frac{1}{h}(U(t,s+h)-U(t,s))u-U(t,s)A(s)u\|_0$$
$$\leq C\|\frac{1}{h}(U(s+h,s)-I)u+A(s)u\|_0+C\|(I-U(s+h,s))A(s)u\|_0.$$

Here, we used the evolutional property and $\|U(t,s+h)\|\leq C$ and $A(s)u\in X_0$ for $u\in D$. □

B The comparison with two formalisms

B1. Lagrangian formulation revisited.

When we treat the problem in the Lagrangian formalism, we have the following theorem:

Theorem B1. *A parametrix of the initial value problem* (1.1) *is given by*

$$\tilde{E}(t,s)u(x)=\tilde{c}_m\int dy\,\tilde{\mu}(t,s,x,y)e^{i\hbar^{-1}\tilde{S}(t,s,x,y)}u(y) \quad \textit{with} \quad \tilde{c}_m=(2\pi i\hbar)^{-m/2}$$
$$=c_m e^{-m\pi i/4}. \tag{B1}$$

Here, $\tilde{S}(t,s)=\tilde{S}(t,s,x,y)$ *satisfies the following Hamilton-Jacobi equation;*

$$\begin{cases} \partial_t\tilde{S}(t,s)+H(t,x,\partial_x\tilde{S}(t,s))=0, \\ \lim_{t\to s}(t-s)\tilde{S}(t,s)=\frac{1}{2}|x-y|^2, \end{cases} \tag{B2}$$

and $\tilde{\mu}(t,s)=\tilde{\mu}(t,s,x,y)$ *satisfies the following continuity equation;*

(B3)
$$\begin{cases} \partial_t\tilde{\mu}(t,s)+\partial_{x_j}\tilde{\mu}(t,s)H_{\xi_j}(t,x,\partial_x\tilde{S}(t,s))+\frac{1}{2}\tilde{\mu}(t,s)\frac{\partial}{\partial x_j}H_{\xi_j}(t,x,\partial_x\tilde{S}(t,s))=0, \\ \lim_{t\to s}(t-s)^{m/2}\tilde{\mu}(t,s)=1. \end{cases}$$

To have this formula (B1), we introduce a classical path $\gamma(\tau,s)=\gamma(\tau,s,x,y)$ which satisfies

(B4)
$$\begin{cases} \frac{d^2}{d\tau^2}\gamma_j(\tau,s)=B_{jk}(\tau,\gamma(\tau,s))\frac{d}{d\tau}\gamma_k(\tau,s)-\partial_t A_j(\tau,\gamma(\tau,s))-\partial_{x_j}V(\tau,\gamma(\tau,s)), \\ \gamma(s,s)=y,\ \gamma(t,s)=x. \end{cases}$$

The unique existence of this path is guaranteed by the assumptions (A) and (V). Then, defining

(B5) $$\tilde{S}(t,s,x,y) = \int_s^t L(\tau,\gamma(\tau,s),\dot{\gamma}(\tau,s))d\tau,$$

we have not only (B2) but also the estimates of $|\partial_x^\alpha \partial_y^\beta \tilde{S}(t,s,x,y)|$ as in [18]. Moreover, it satisfies

(B6) $$\partial_s \tilde{S}(t,s) - H(s,y,-\partial_y \tilde{S}(t,s)) = 0.$$

Defining

$$\tilde{\mu}(t,s,x,y) = \left[\det\left(\frac{\partial^2 \tilde{S}(t,s,x,y)}{\partial x_j \partial y_k}\right)\right]^{1/2},$$

we have a solution of (B3) with estimates $|\partial_x^\alpha \partial_y^\beta (\tilde{\mu}(t,s,x,y)-1)|$, and which satisfies also

(B7)
$$\partial_s \tilde{\mu}(t,s) - \partial_{y_k}\tilde{\mu}(t,s) H_{\xi_k}(s,y,-\partial_y \tilde{S}(t,s)) - \frac{1}{2}\tilde{\mu}(t,s)\frac{\partial}{\partial y_k} H_{\xi_k}(s,y,-\partial_y \tilde{S}(t,s)) = 0.$$

Proposition B2.

(B8)
$$\frac{\partial}{\partial t}\tilde{E}(t,s)u + \mathbb{H}(t,x,D_x^\hbar)\tilde{E}(t,s)u = \tilde{G}_L(t,s)u, \quad \textit{with} \quad \|\tilde{G}_L(t,s)u\| \le C\hbar^2|t-s|\|u\|.$$

Proof. In fact, using the differentiation under the oscillatory integral sign and applying (B2) and (B3), we have readily

$$\tilde{G}_L(t,s)u(x) = \hbar^2 \int dy\, \Delta_x \tilde{\mu}(t,s,x,y) e^{i\hbar^{-1}\tilde{S}(t,s,x,y)} u(y).$$

As $|\Delta_x \tilde{\mu}(t,s,x,y)| \le C|t-s|$, etc., we have the desired result. □

Proposition B3.

(B9)
$$\frac{\partial}{\partial s}\tilde{E}(t,s)u - \tilde{E}(t,s)\mathbb{H}(s,y,D_y^\hbar)u = \tilde{G}_R(t,s)u \quad \textit{with} \quad \|\tilde{G}_R(t,s)u\| \le C\hbar^2|t-s|\|u\|.$$

Proof. By the integration by parts under the oscillatory integral sign, we have

$$\int dy\,\tilde{\mu}(t,s,x,y)e^{i\hbar^{-1}\tilde{S}(t,s,x,y)}\mathbb{H}(s,y,D_y^{\hbar})u(y)$$
$$= \int dy\,\Big[\frac{1}{2}\Big(\frac{\hbar}{i}\frac{\partial}{\partial y_j} + A_j(s,y)\Big)^2 - V(s,y)\Big]\big(\tilde{\mu}(t,s,x,y)e^{i\hbar^{-1}\tilde{S}(t,s,x,y)}\big)\,u(y).$$

On the other hand, we have

$$\frac{\hbar}{i}\frac{\partial}{\partial s}\tilde{E}(t,s)u = \int dy\,\frac{\hbar}{i}\frac{\partial}{\partial s}\big(\tilde{\mu}(t,s,x,y)e^{i\hbar^{-1}\tilde{S}(t,s,x,y)}\big)\,u(y).$$

As is shown before,

$$\frac{\partial}{\partial s}\big(\tilde{\mu}(t,s)e^{i\hbar^{-1}\tilde{S}(t,s)}\big) = \big(\tilde{\mu}_s(t,s) + i\hbar^{-1}\tilde{S}_s(t,s)\tilde{\mu}(t,s)\big)e^{i\hbar^{-1}\tilde{S}(t,s)},$$

applying (B6) and (B7), we get readily that

$$\tilde{G}_R(t,s)u(x) = \hbar^2\int dy\,\Delta_y\tilde{\mu}(t,s,x,y)e^{i\hbar^{-1}\tilde{S}(t,s,x,y)}u(y).$$

□

From these propositions, we have

Proposition B4.

$$\|\tilde{E}(t,s)\tilde{E}(s,r) - \tilde{E}(t,r)\| \le C\hbar(|t-s|^2 + |s-r|^2), \tag{B10}$$
$$\|\tilde{E}(s,t)^*\tilde{E}(s,r) - \tilde{E}(t,r)\| \le C\hbar(|t-s|^2 + |s-r|^2). \tag{B11}$$

B2. The difference.

(1) In calculating (4.13) and (4.14), we derive an operator $\hat{H}^W(t,x,D_x^{\hbar})$ from $H(t,x,\xi)$ using the Fourier transformation. While proving (B10) and (B11), we use $\mathbb{H}(t,x,D_x^{\hbar})$ as a given operator without considering from where it stemms.

(2) In the Lagrangian formulation, the time reversing and taking the adjoint are rather nicely related. To show this, we have

Proposition B5. *Under Assumptions* (A) and (V), *we have*

$$\tilde{S}(t,s,x,y) = -\tilde{S}(s,t,y,x). \tag{B12}$$

Proof. Putting $x = \bar{x},\ y = \underline{x}$, we use the results in §2. Let $q(\tau)$ be a solution of (B4) with $q(s) = \underline{x},\ q(t) = \bar{x}$ where τ moves from s to t. Then,

$$\tilde{S}(t, s, \bar{x}, \underline{x}) = \int_s^t d\tau\, L(\tau, q(\tau), v(\tau)) \text{ with } v(\tau) = \dot{q}(\tau). \tag{B13}$$

Using the change of variable $\tau = s + \theta(t - s)$ with $0 \le \theta \le 1$, we have

$$\tilde{S}(t, s, \bar{x}, \underline{x}) = (t - s) \int_0^1 d\theta\, L(s + \theta(t - s), q(s + \theta(t - s)), v(s + \theta(t - s))).$$

Moreover, for $\gamma_j(\theta) = q_j(s + \theta(t - s))$, we have

(B14)

$$\begin{cases} (t-s)^2 \dfrac{d^2}{d\theta^2}\gamma_j(\theta) = (t - s)B_{jk}(s + \theta(t - s), \gamma(\theta))\dfrac{d}{d\theta}\gamma_k(\theta) \\ \qquad - (t - s)^2 \partial_t A_j(s + \theta(t - s), \gamma(\theta)) - (t - s)^2 \partial_{x_j} V(s + \theta(t - s), \gamma(\theta)), \\ \gamma(0) = \underline{x},\ \gamma(1) = \bar{x}. \end{cases}$$

Analogously, let $\tilde{q}(\tilde{\tau})$ satisfy (B4) with $\tilde{q}(t) = \bar{x},\ \tilde{q}(s) = \underline{x}$ where $\tilde{\tau}$ moves from t to s. Then, by putting $\tilde{\tau} = t + (1 - \theta)(s - t) = s + \theta(t - s)$, we have

(B15)

$$\tilde{S}(s, t, \underline{x}, \bar{x}) = -(t - s) \int_0^1 d\theta\, L(s + \theta(t - s), \tilde{q}(s + \theta(t - s)), \tilde{v}(s + \theta(t - s)).$$

It is easily checked that $\tilde{\gamma}(\theta) = \tilde{q}(s + \theta(t - s))$ satisfies the same equation as (B14). By the uniqueness of the solution of (B14), we have the desired result. □

Therefore, combining above with the definition of $\tilde{\mu}(t, s, x, y)$, we have

Corollary B6.

$$\tilde{\mu}(t, s, x, y) = \tilde{\mu}(t, s, y, x) = (-1)^{m/2}\tilde{\mu}(s, t, y, x).$$

Now, we have

Proposition B7. *Under these circumstance, we have*

$$\tilde{E}(t, s)^* = \tilde{E}(s, t). \tag{B16}$$

Proof. We have readily

$$\text{(B17)}\qquad \begin{aligned} \tilde{E}(t,s)^*v(x) &= \overline{\tilde{c}_m}\int dy\,\overline{\tilde{\mu}(t,s,y,x)}e^{-i\hbar^{-1}\tilde{S}(t,s,y,x)}v(y) \\ &= \tilde{c}_m\int dy\,\tilde{\mu}(t,s,y,x)e^{i\hbar^{-1}\tilde{S}(s,t,x,y)}v(y) = \tilde{E}(s,t)v(x). \end{aligned}$$

In fact, $\overline{\tilde{c}_m}\overline{\tilde{\mu}(t,s,y,x)} = \tilde{c}_m\tilde{\mu}(s,t,x,y)$ follows from directly. □

REMARKS. (1) In this formulation, we have (B10) from (B11) and (B16) without calculating (B9).
(2) If we knew the uniqueness of the solution of (B2), we had (B12) combining (B2) and (B6).

But in the Hamiltonian formulation, this relation does not seem to hold in general. We have the representation

$$\text{(B18)}\qquad E(t,s)^*v(x) = c_m^2\iint d\xi\,dy\,\overline{\mu(t,s,y,\xi)}e^{i\hbar^{-1}(x\cdot\xi - S(t,s,y,\xi))}v(y).$$

Using (4.14) and the proof of Proposition 5.4 of [6], we have

$$\|E(t,s)^*v - E(t,s)^{-1}v\| \le C|t-s|^2\|v\|,$$

and by (5.9),

$$\|E(s,t)v - E(t,s)^{-1}v\| \le C|t-s|^2\|v\|.$$

This yields at least

Proposition B8.

$$\text{(B19)}\qquad \|E(t,s)^* - E(s,t)\| \le C|t-s|^2.$$

B3. Problems.

(i) In [7], Fujiwara gives a kernel representation of the fundamental solution of (1.1). There appears the Maslov index. From the definition of the Maslov index, it seems natural to formulate the kernel representation in the phase space, in other word, the Hamiltonian path-integral will be helpfull to understand the appearance of the Maslov index.

(ii) In the Lagrangian formulation, we have (B10) with the explicit dependence of $\hbar$. But, we have not such explicit dependence in (5.9) for the time being.

(iii) The singularity w.r.t $t-s$ or others in $S(t,s,\cdots)$ or $\mu(t,s,\cdots)$ diminishes in the Hamiltonian formulation comparing with the Lagrangian one. As an example, we consider the Hamiltonian $H(x,\xi)=\frac{1}{2}(\xi-ax)^2+\frac{1}{2}b^2x^2$, and then we have

$$\tilde{S}(t,0,x,y)=\frac{b}{2}(\cot bt)(x^2+y^2)-\frac{b}{\sin bt}xy+\frac{a}{2}(x^2-y^2),\ \tilde{\mu}(t,0,x,y)=\frac{b}{\sin bt},$$
$$S(t,0,x,\xi)=\frac{2bx\xi-(\xi^2+(a^2+b^2)x^2)\sin bt}{2(b\cos bt-a\sin bt)},\ \mu(t,0,x,\xi)=\frac{b}{b\cos bt-a\sin bt}.$$

More precisely, the singularity at time $t=0$ of $\tilde{\mu}(t,0,x,y)$ stems from the delta function character when $t\to 0$ in the Lagrangian formulation. But in the Hamiltonian one, there is no singularity for $\mu(t,0,x,\xi)$ when $t=0$.

On the other hand, Yajima [19] claims that there exists no smooth fundamental solution for the Schrödinger operator with time independent super-quadratic potential in $\mathbb{R}^1$, e.g. $\frac{\hbar}{i}\frac{\partial}{\partial t}-\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}+x^4$. From Yajima's interpretation, this is because for any spatial points x and y and any time t, there are trajectories with arbitrarily high energy that leave y at time zero and reach x at time t.

Therefore, we want to ask even after Yajima's claim whether we have a fundamental solution for the above operator in the form

$$\int d\xi\,\mu(t,0,x,\xi)e^{i\hbar^{-1}S(t,0,x,\xi)}\hat{u}(\xi)$$

with smooth functions $S(t,0,x,\xi)$ and $\mu(t,0,x,\xi)$?

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Department of Mathematics,
Tokyo Institute of Technology,
Oh-okayama, Meguro-ku, Tokyo, 152, Japan